Access DB# ___________

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Kahsay Habte   Examiner # : 78271   Date: May 14/03
Art Unit: 1624   Phone Number 308-4717   Serial Number: 10/049,205
Mail Box and Bldg/Room Location: 4D-16   Results Format Preferred (circle): PAPER DISK E-MAIL
4E-12

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Process of catalyzing the oxidation of Organic Compound

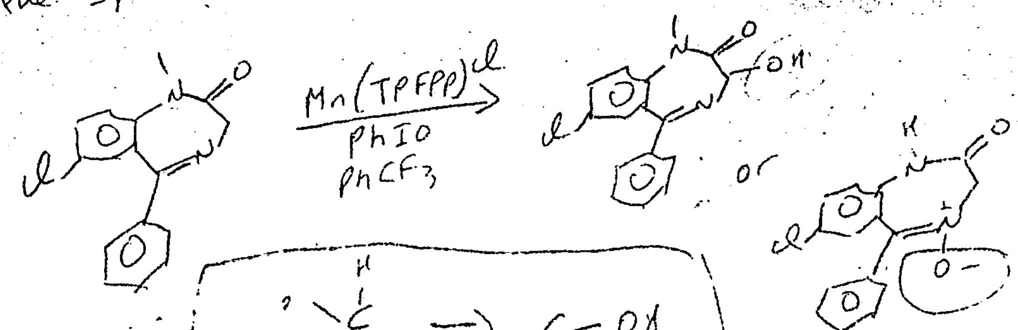
Inventors (please provide full names): Patrick Bernadelli

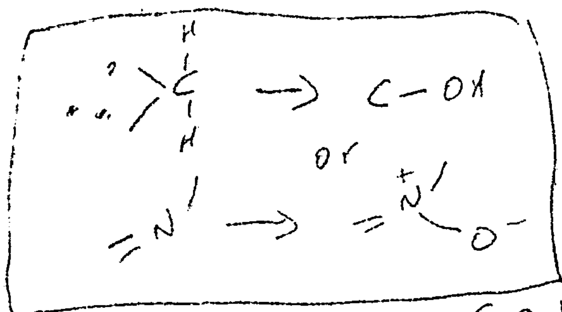
Earliest Priority Filing Date: 08/10/1999

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search for any process where any metalloporphyrin is used as "oxidation catalyst" in the presence of aprotic solvent

In the specification, they have specific example





Point of Contact.
Barb O'Bryen
Technical Information Specialist
STIC CM1 6A05 308-4291

See WO 96/08455 as a prior art

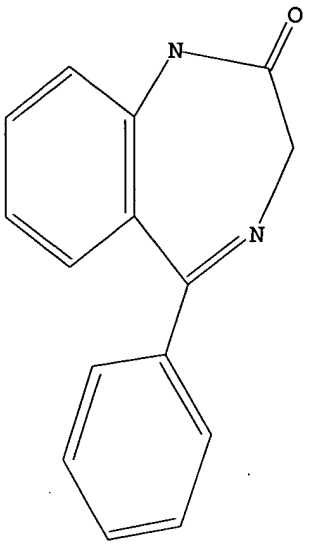
****

STAFF USE ONLY	**Type of Search**	**Vendors and cost where applicable**
Searcher:	NA Sequence (#)	STN
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#) 3	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed: 5-15-03	Litigation	Lexis/Nexis
Searcher Prep & Review Time:	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time: 15 / 30	Other	Other (specify)

PTO-1590 (1-2000)

L Number	Hits	Search Text	DB	Time stamp
1	761	540/145, 540/504	USPAT	2003/05/14 10:32
2	306	(540/145, 540/504) and oxidation$	USPAT	2003/05/14 10:33
3	4	540/145 and diazepam$	USPAT	2003/05/14 10:35
5	371	(540/145, 540/504) and cataly$	USPAT	2003/05/14 10:36
6	239	((540/145, 540/504) and cataly$) and oxidation	USPAT	2003/05/14 10:36
7	5	(((540/145, 540/504) and cataly$) and oxidation) and diazepam$	USPAT	2003/05/14 10:36

L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 615 TO ITERATE

100.0% PROCESSED 615 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 10813 TO 13787
PROJECTED ANSWERS: 8212 TO 10828

L2 50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:05:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11792 TO ITERATE

100.0% PROCESSED 11792 ITERATIONS 9263 ANSWERS
SEARCH TIME: 00.00.01

L3 9263 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 148.15 148.36

FILE 'CAPLUS' ENTERED AT 10:05:47 ON 14 MAY 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 May 2003 VOL 138 ISS 20
FILE LAST UPDATED: 13 May 2003 (20030513/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 18623 L3

=> s l4 and (preparation or oxidation?)
L5 2755 L4 AND (PREPARATION OR OXIDATION?)

=> s l5 and (?porphyrin?)
L6 3 L5 AND (?PORPHYRIN?)

=> d ibib abs hitstr tot

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:115086 CAPLUS
DOCUMENT NUMBER: 134:178573
TITLE: Process for the **metalloporphyrin** catalyzed **oxidation** of organic compounds
INVENTOR(S): Bernardelli, Patrick
PATENT ASSIGNEE(S): Warner Lambert Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

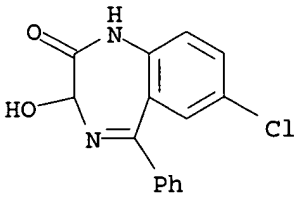
JP 2003506419 T2 20030218 JP 2001-515270 20000809
PRIORITY APPLN. INFO.: US 1999-148079P P 19990810
US 1999-150101P P 19990820
WO 2000-EP7726 W 20000809

OTHER SOURCE(S): CASREACT 134:178573

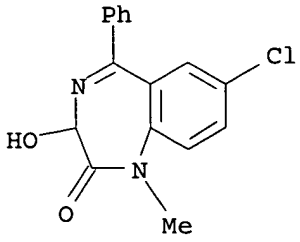
AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of **metalloporphyrin** (tetrakis(**pentafluorophenylporphyrin**)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, aprotic, polyhalogenated solvent (benzotrifluoride). **Oxidn.** of diazepam is conducted to mimic **oxidn.** (metab.) in biol. systems. The products of the **oxidn.** of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert aprotic solvent shows improved **oxidn.** yields when compared to prior art (e.g., CH3CN-CH2Cl2-water mixts.).

IT **604-75-1P 846-50-4P 963-39-3P**
1088-11-5P 2888-64-4P
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(process for **metalloporphyrin**-catalyzed **oxidn.** of org. compds.)

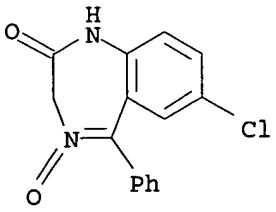
RN 604-75-1 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



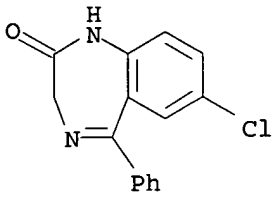
RN 846-50-4 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



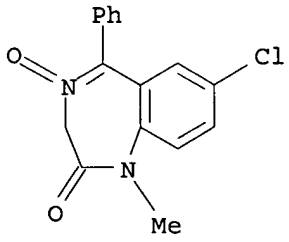
RN 963-39-3 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-, 4-oxide (7CI, 8CI, 9CI) (CA INDEX NAME)



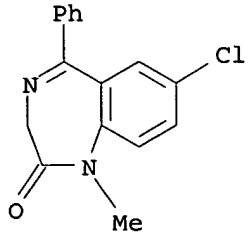
RN 1088-11-5 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl- (8CI, 9CI) (CA INDEX NAME)

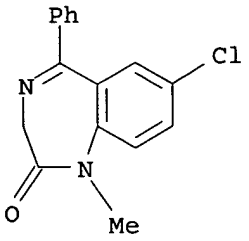


RN 2888-64-4 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-, 4-oxide (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **439-14-5**, Diazepam
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for **metalloporphyrin**-catalyzed **oxidn**. of org. compds.)
RN 439-14-5 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl- (8CI, 9CI) (CA INDEX NAME)





REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:766507 CAPLUS
DOCUMENT NUMBER: 130:29221
TITLE: **Preparation** of solid porous matrixes for pharmaceutical uses
INVENTOR(S): Unger, Evan C.
PATENT ASSIGNEE(S): ImaRx Pharmaceutical Corp., USA
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

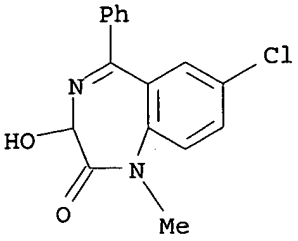
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9851282	A1	19981119	WO 1998-US9570	19980512
W: AU, BR, CA, CN, JP, KR, NZ				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 2002039594	A1	20020404	US 1998-75477	19980511
AU 9873787	A1	19981208	AU 1998-73787	19980512
EP 983060	A1	20000308	EP 1998-921109	19980512
R: DE, FR, GB, IT, NL				
US 2001018072	A1	20010830	US 2001-828762	20010409

PRIORITY APPLN. INFO.: US 1997-46379P P 19970513
US 1998-75477 A 19980511
WO 1998-US9570 W 19980512

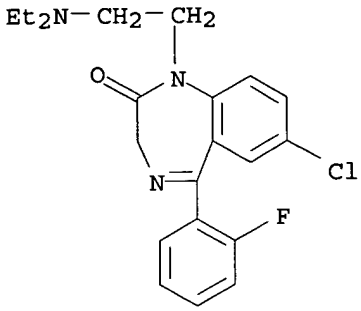
AB A solid porous matrix formed from a surfactant, a solvent, and a bioactive agent is described. Thus, amphotericin nanoparticles were prepd. by using ZrO2 beads and a surfactant. The mixt. was milled for 24 h.

IT **846-50-4**, Temazepam **1172-18-5**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**prepn**. of solid porous matrixes for pharmaceutical uses)

RN 846-50-4 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-1-methyl-5-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 1172-18-5 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1-[2-(diethylamino)ethyl]-5-(2-fluorophenyl)-1,3-dihydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

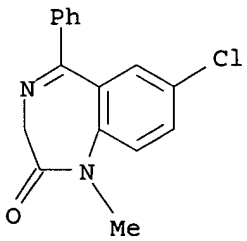
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:255694 CAPLUS
DOCUMENT NUMBER: 129:23391
TITLE: Evidence for the existence of [3H]-trimetazidine binding sites involved in the regulation of the mitochondrial permeability transition pore
AUTHOR(S): Morin, Didier; Elimadi, Aziz; Sapena, Rosa; Crevat, Aime; Carrupt, Pierre-Alain; Testa, Bernard; Tillement, Jean-Paul
CORPORATE SOURCE: Departement de Pharmacologie, IM3, Faculte de Medecine de Paris XII, Creteil, F-94010, Fr.
SOURCE: British Journal of Pharmacology (1998), 123(7), 1385-1394
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Trimetazidine is an anti-ischemic drug effective in different exptl. models but its mechanism of action is not fully understood. Data indicate that mitochondria could be the main target of this drug. The aim of this work was to investigate the binding of [3H]-trimetazidine on a purified **prepn**. of rat liver mitochondria. [3H]-trimetazidine binds to two

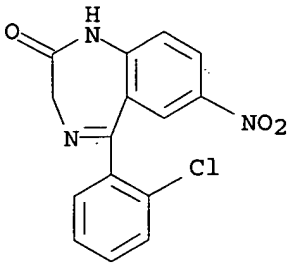
populations of mitochondrial binding sites with Kd values of 0.96 and 84 .mu.M. The total concn. of binding sites is 113 pmol mg-1 protein. Trimetazidine binding sites are differently distributed. The high-affinity ones are located on the outer membranes and represent only a small part (4%) of total binding sites, whereas the low-affinity ones are located on the inner membranes and are more abundant (96%) with a Bmax = 108 pmol mg-1 protein. Drug displacement studies with pharmacol. markers for different mitochondrial targets showed that [3H]-trimetazidine binding sites are different from previously described mitochondrial sites. The possible involvement of [3H]-trimetazidine binding sites in the regulation of the mitochondrial permeability transition pore (MTP), a voltage-dependent channel sensitive to cyclosporin A, was investigated with mitochondrial swelling expts. Trimetazidine inhibited the mitochondrial swelling induced by Ca2+ plus tert-butylhydroperoxide (t-BH). This effect was concn.-dependent with an IC50 value of 200 .mu.M. Assuming that trimetazidine effectiveness may be related to its structure as an amphiphilic cation, the authors compared it with other compds. exhibiting the same chem. characteristic both for their ability to inhibit MTP opening and to displace [3H]-trimetazidine bound to mitochondria. Selected compds. were drugs known to interact with various biol. membranes. A strong correlation between swelling inhibition potency and low-affinity [3H]-trimetazidine binding sites was obsd.: r=0.907. These data suggest that mitochondrial sites labeled with [3H]-trimetazidine may be involved in the MTP inhibition.

IT **439-14-5**, Diazepam **1622-61-3**, Clonazepam
1622-62-4, Flunitrazepam
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(evidence for existence of [3H]-trimetazidine binding sites involved in regulation of mitochondrial permeability transition pore and effect of other agents in relation to anti-ischemic activity)

RN 439-14-5 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 1622-61-3 CAPLUS
CN 2H-1,4-Benzodiazepin-2-one, 5-(2-chlorophenyl)-1,3-dihydro-7-nitro- (9CI) (CA INDEX NAME)



RN 1622-62-4 CAPLUS
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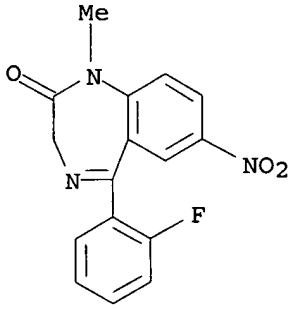


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	20.03	168.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.95	-1.95

STN INTERNATIONAL LOGOFF AT 10:07:37 ON 14 MAY 2003

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 10:22:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3593 TO ITERATE

27.8% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 68267 TO 75453
PROJECTED ANSWERS: 59096 TO 65796

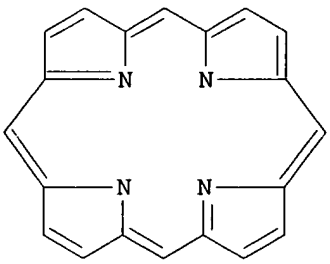
L2 50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:22:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 73285 TO ITERATE

100.0% PROCESSED 73285 ITERATIONS 64039 ANSWERS
SEARCH TIME: 00.00.01

L3 64039 SEA SSS FUL L1

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 148.55 148.76

FILE 'CAPLUS' ENTERED AT 10:22:52 ON 14 MAY 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 May 2003 VOL 138 ISS 20
FILE LAST UPDATED: 13 May 2003 (20030513/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 42453 L3

=> s l4 and oxidation?
L5 5826 L4 AND OXIDATION?

=> s l5 and (aprotic?)
L6 45 L5 AND (APROTIC?)

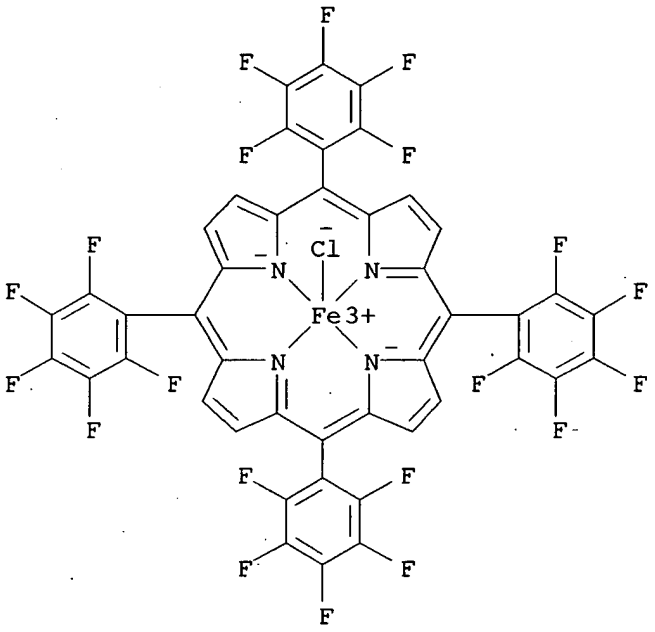
=> d ibib abs hitstr tot

L6 ANSWER 1 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:675277 CAPLUS
DOCUMENT NUMBER: 138:153305
TITLE: Remarkable solvent effect on the yield and specificity of **oxidation** of naphthalene catalyzed by iron(III) porphyrins
AUTHOR(S): Khavasi, Hamid Reza; Hosseiny Davarani, S. Saeed; Safari, Nasser
CORPORATE SOURCE: Chemistry Department, Shahid Beheshti University, Evin, Tehran, 19839, Iran
SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 188(1-2), 115-122
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153305
AB **Oxidn**. of naphthalene was performed with tetrakis(pentafluorophenyl)porphyrin iron(III) chloride (F20TPPFeIIICl) or tetrakis(2,6-dichlorophenyl)porphyrin iron(III) chloride (TDCPPFeIIICl) or tetramesitylporphyrin iron(III) chloride (TMPFeIIICl) as catalyst and m-chloroperbenzoic acid or pentafluoroiodosylbenzene or tert-Bu hydroperoxide as oxidant in different media in the presence of imidazole as cocatalyst. In an **aprotic** solvent (CH3CN:CH2Cl2 1:1) and in the presence of F20TPPFeIIICl, 1-naphthol, 2-naphthol and 1,4-naphthoquinone yields based on m-chloroperbenzoic acid oxidant were 77.7, 2.1 and 5.6%, resp. The best yield for 1,4-naphthoquinone occurred in methanol with F20TPPFeIIICl and was 52.8%. The effect of bases on the yield and specificity of the naphthalene **oxidn**. were studied. When imidazole was changed to pyridine in F20TPPFeIIICl, the yield of

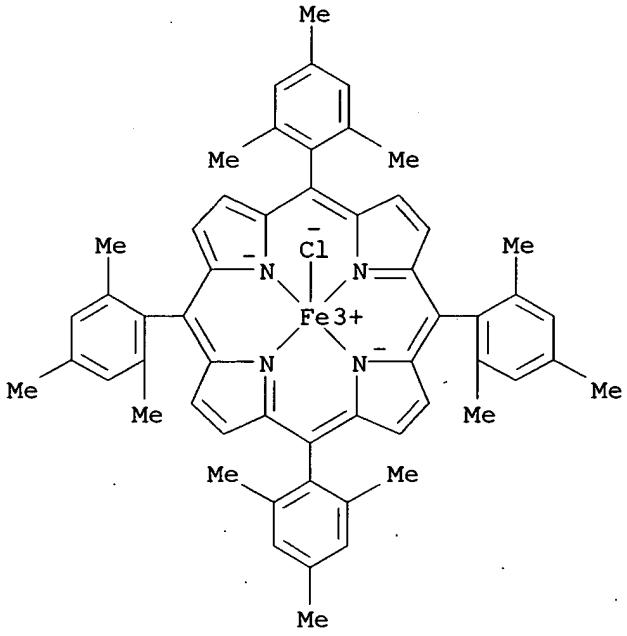
1-naphthol decreased from 77.7 to 55.3%, whereas for TDCPPFeIIICl catalyst, the yield changed from 61.1 to 18.3%.

IT **36965-71-6 77439-21-5 91042-27-2**
RL: CAT (Catalyst use); USES (Uses)
(solvent effect on **oxidn**. of naphthalene to naphthols and naphthoquinone catalyzed by iron(III) porphyrins)

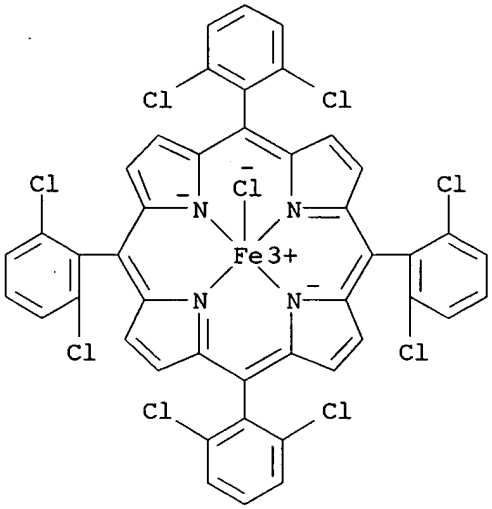
RN 36965-71-6 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



RN 77439-21-5 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-(9CI) (CA INDEX NAME)



RN 91042-27-2 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:301156 CAPLUS
DOCUMENT NUMBER: 137:56469
TITLE: Effects of Solvents on the Electron Configurations of

the Low-Spin Dicyano[meso-tetrakis(2,4,6-triethylphenyl)porphyrinato]iron(III) Complex: Importance of the C-H.cntdot..cntdot..cntdot.N Weak Hydrogen Bonding

AUTHOR(S): Ikezaki, Akira; Nakamura, Mikio
CORPORATE SOURCE: Department of Chemistry, Toho University School of Medicine, Ota-ku Tokyo, 143-8540, Japan

SOURCE: Inorganic Chemistry (2002), 41(10), 2761-2768
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:56469

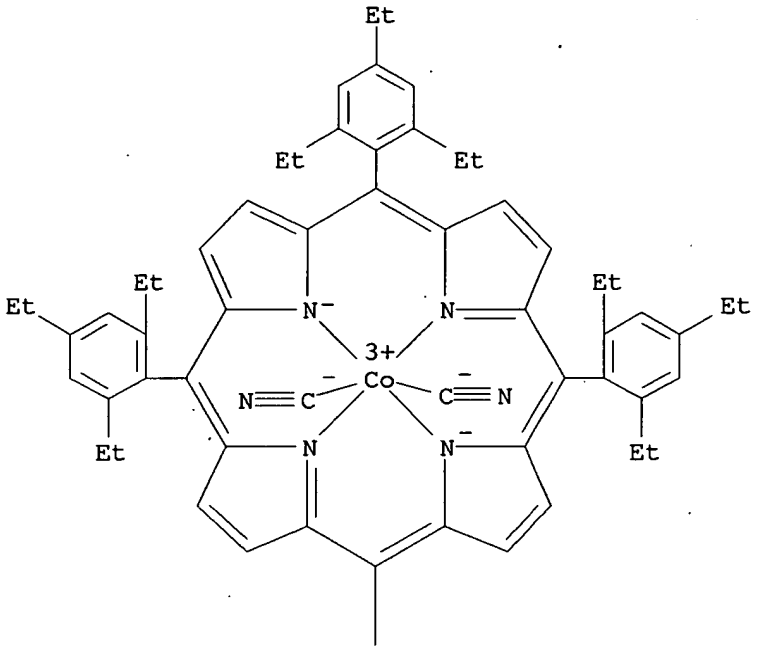
AB There are two types of electron configurations, (dxy)2(dxz,dyz)3 and (dxz,dyz)4(dxy)1, in low-spin Fe(III) porphyrin complexes. To reveal the solvent effects on the ground-state electron configurations, the authors have examd. the 13C- and 1H-NMR spectra of low-spin dicyano[meso-tetrakis(2,4,6-triethylphenyl)porphyrinato]ferrate(III) in a variety of solvents, including protic, dipolar **aprotic**, and nonpolar solvents. From the NMR study, the authors have reached the following conclusions: (i) the complex adopts the ground state with the (dxz,dyz)4(dxy)1 electron configuration, the (dxz,dyz)4(dxy)1 ground state, in MeOH, because the d.pi. orbitals are stabilized due to the O-H.cntdot..cntdot..cntdot.N H bonding between the coordinated cyanide and MeOH; (ii) the complex also exhibits the (dxz,dyz)4(dxy)1 ground state in nonpolar solvents, such as CHCl3 and CH2Cl2, which is ascribed to the stabilization of the d.pi. orbitals due to the C-H.cntdot..cntdot..cntdot.N weak H bonding between the coordinated cyanide and the solvent mols.; (iii) the complex favors the (dxz,dyz)4(dxy)1 ground state in dipolar **aprotic** solvents, such as DMF, DMSO, and acetone, though the (dxz,dyz)4(dxy)1 character is less than that in CHCl3 and CH2Cl2; (iv) the complex adopts the (dxy)2(dxz,dyz)3 ground state in nonpolar solvents, such as toluene, benzene, and tetrachloromethane, because of the lack of H bonding in these solvents; (v) MeCN behaves like nonpolar solvents, such as toluene, benzene, and tetrachloromethane, though it is classified as a dipolar **aprotic** solvent. Although the NMR results were interpreted in terms of the solvent effects on the ordering of the dxy and d.pi. orbitals, they could also be interpreted in terms of the solvent effects on the population ratios of two isomers with different electron configurations. In fact, the authors obsd. the unprecedented EPR spectra at 4.2 K which contain both the axial- and large gmax-type signals in some solvents such as benzene, toluene, and MeCN. The observation of the two types of signals was ascribed to the slow interconversion on the EPR time scale at 4.2 K between the ruffled complex with the (dxz, dyz)4(dxy)1 ground state and, possibly, the planar (or nearly planar) complex with the (dxy)2(dxz, dyz)3 ground state.

IT **172354-92-6P**, (Tetrakis(2,4,6-triethylphenyl)porphyrinato)cobalt
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and **oxidn.** of)

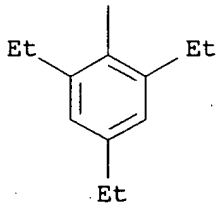
RN 172354-92-6 CAPLUS

CN Cobalt, [5,10,15,20-tetrakis(2,4,6-triethylphenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

PAGE 1-A

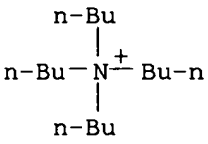


PAGE 2-A



CM 2

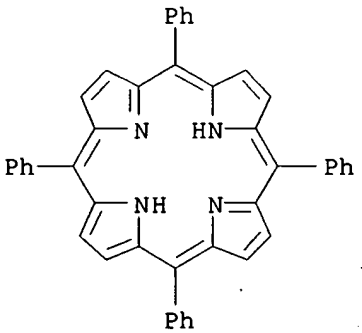
CRN 10549-76-5
CMF C16 H36 N



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:291936 CAPLUS
DOCUMENT NUMBER: 135:129453
TITLE: Solvent effects on the sensitized photoxygenation of lidocaine
AUTHOR(S): Zanocco, A. L.; Lemp, E.; Pizarro, N.; de la Fuente, J. R.; Gunther, G.
CORPORATE SOURCE: Departamento de Quimica Organica y Fisicoquimica, Facultad de Ciencias Quimicas y Farmaceuticas, Casilla 233, Santiago-1, Universidad de Chile, Santiago, Chile
SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2001), 140(2), 109-115
CODEN: JPPCEJ; ISSN: 1010-6030
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Detection of O2(1.DELTA.g) phosphorescence emission, .lambda.max=1270 nm, following laser excitation and steady state methods were employed to det. both the total const., kTLID, and the chem. reaction rate consts., kRLID, for reaction between the anesthetic lidocaine and singlet O in several solvents. Values of kTLID range from 0.20 .+-. 0.09 .times. 106 M-1 s-1 in trifluoroethanol to 45.8 .+-. 2.40 .times. 106 M-1 s-1 in N,N-dimethylacetamide. Values of kRLID are .gtoreq.1 order of magnitude lower than kTLID values in a given solvent. Solvent effect on quenching rates shows that reaction mechanism involves formation of a charge transfer exciplex. Correlation of kTLID values with solvent parameters does not follow that obsd. for a typical tertiary amine such as NEt3. Although kTLID values are lower in H bond donor solvents, this solvent effect is significantly smaller than that for NEt3, and no expected decrease in lidocaine reactivity with change from **aprotic** to protic solvents was found. This result is ascribed to weaker H bonding between the amino moiety in lidocaine and the solvent. Otherwise, H bond acceptor solvents increase kTLID to a greater extent than that NEt3. This can be explained by intra-mol. H bonding or electrostatic interactions that stabilize lidocaine and H bond acceptor solvents disrupt these interactions.
IT **917-23-7**, 5,10,15,20-Tetraphenylporphine
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(sensitizer; kinetic results of sensitized photooxygenation of lidocaine using both steady-state and time-resolved methods)
RN 917-23-7 CAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:115086 CAPLUS
DOCUMENT NUMBER: 134:178573
TITLE: Process for the metalloporphyrin catalyzed **oxidation** of organic compounds
INVENTOR(S): Bernardelli, Patrick
PATENT ASSIGNEE(S): Warner Lambert Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809

PRIORITY APPLN. INFO.: US 1999-148079P P 19990810
US 1999-150101P P 19990820
WO 2000-EP7726 W 20000809

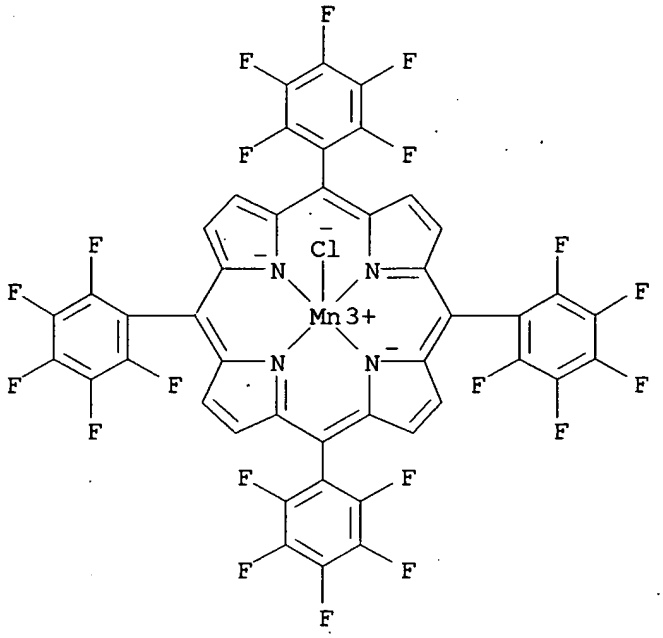
OTHER SOURCE(S): CASREACT 134:178573

AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, **aprotic**, polyhalogenated solvent (benzotrifluoride). **Oxidn.** of diazepam is conducted to mimic **oxidn.** (metab.) in biol. systems. The products of the **oxidn.** of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert **aprotic** solvent shows improved **oxidn.** yields when compared to prior art (e.g., CH3CN-CH2Cl2-water mixts.).

IT **79968-43-7**
RL: CAT (Catalyst use); USES (Uses)
(process for metalloporphyrin-catalyzed **oxidn.** of org. compds.)

RN 79968-43-7 CAPLUS
CN Manganese, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-).kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-

(9CI) (CA INDEX NAME)



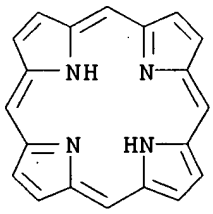
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:695736 CAPLUS
DOCUMENT NUMBER: 133:360395
TITLE: First success of catalytic epoxidation of olefins by an electron-rich iron(III) porphyrin complex and H2O2: imidazole effect on the activation of H2O2 by iron porphyrin complexes in **aprotic** solvent
AUTHOR(S): Nam, Wonwoo; Lee, Ha J.; Oh, So-Young; Kim, Cheal; Jang, Ho G.
CORPORATE SOURCE: Department of Chemistry, Division of Molecular Life Sciences, Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Journal of Inorganic Biochemistry (2000), 80(3-4), 219-225
CODEN: JIBIDJ; ISSN: 0162-0134
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:360395
AB An electron-rich iron(III) porphyrin complex (meso-tetramesitylporphinato)iron(III) chloride [Fe(TMP)Cl], was found to catalyze the epoxidn. of olefins by aq. 30% H2O2 when the reaction was carried out in the presence of 5-chloro-1-methylimidazole (5-Cl-1-MeIm) in **aprotic** solvent. Epoxides were the predominant products with trace amts. of allylic **oxidn**. products, indicating that Fenton-type **oxidn**. reactions were not involved in the olefin epoxidn. reactions. Cis-Stilbene was stereospecifically oxidized to

cis-stilbene oxide without giving isomerized trans-stilbene oxide product, demonstrating that neither hydroperoxy radical (HOO.cntdot.) nor oxoiron(IV) porphyrin [(TMP)FeIV=O] was responsible for the olefin epoxidns. We also found that the reactivities of other iron(III) porphyrin complexes such as (meso-tetrakis(2,6-dichlorophenyl)porphinato)iron(III) chloride [Fe(TDCPP)Cl], (meso-tetrakis(2,6-difluorophenyl)porphinato)iron(III) chloride [Fe(TDFPP)Cl], and (meso-tetrakis(pentafluorophenyl)porphinato)iron(III) chloride [Fe(TPFPP)Cl] were significantly affected by the presence of the imidazole in the epoxidn. of olefins by H2O2. These iron porphyrin complexes did not yield cyclohexene oxide in the epoxidn. of cyclohexene by H2O2 in the absence of 5-Cl-1-MeIm in **aprotic** solvent; however, addn. of 5-Cl-1-MeIm to the reaction solns. gave high yields of cyclohexene oxide with the formation of trace amts. of allylic **oxidn**. products. We proposed, on the basis of the results of mechanistic studies, that the role of the imidazole is to decelerate the O-O bond cleavage of an iron(III) hydroperoxide porphyrin (or H2O2-iron(III) porphyrin adduct) and that the intermediate transfers its oxygen to olefins prior to the O-O bond cleavage.

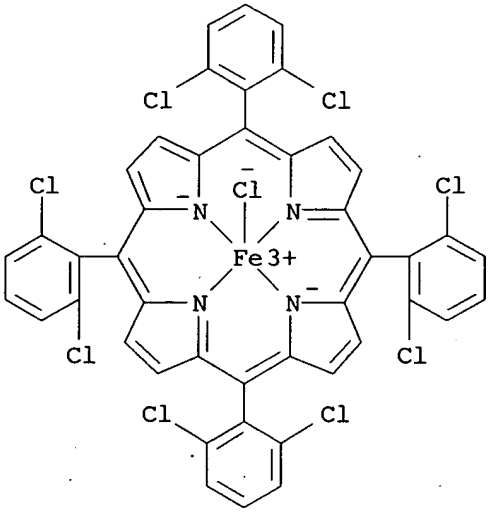
IT **101-60-0D**, Porphyrin, iron complexes **36965-71-6**, (meso-Tetrakis(pentafluorophenyl)porphinato)iron(III) chloride **77439-21-5 91042-27-2**, (meso-Tetrakis(2,6-dichlorophenyl)porphinato)iron(III) chloride **99038-25-2**, (meso-Tetrakis(2,6-difluorophenyl)porphinato)iron(III) chloride
RL: CAT (Catalyst use); USES (Uses)
(catalytic epoxidn. of olefins by electron-rich iron(III) porphyrin complexes and hydrogen peroxide in presence of chloromethylimidazole in **aprotic** solvent)

RN 101-60-0 CAPLUS
CN 21H,23H-Porphine (9CI) (CA INDEX NAME)

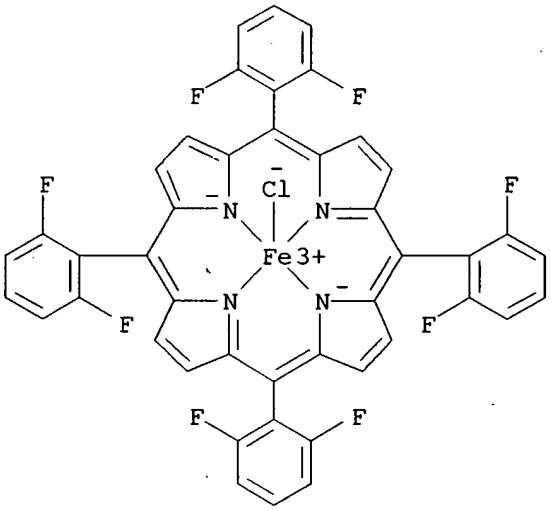


RN 36965-71-6 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

INDEX NAME)



RN 99038-25-2 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(2,6-difluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:675094 CAPLUS
DOCUMENT NUMBER: 133:362488
TITLE: Reaction of Singlet Oxygen with trans-4-Propenylanisole. Formation of [2 + 2] Products with

Added Acid

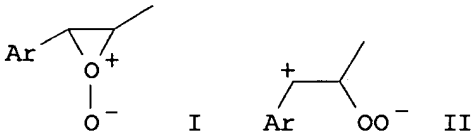
AUTHOR(S): Greer, Alexander; Vassilikogiannakis, Georgios; Lee, Kun-Chun; Koffas, Telly S.; Nahm, Keepyung; Foote, Christopher S.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095, USA

SOURCE: Journal of Organic Chemistry (2000), 65(21), 6876-6878
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:362488

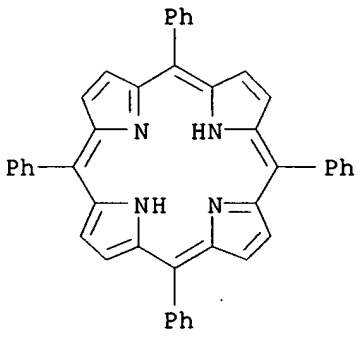
GI



AB The authors report the effects of added acid in the reaction of singlet O with trans-4-propenylanisole (1). The authors provide evidence that solvent acidity modifies the behavior of the transient intermediates. Relative to reactions in **aprotic** solvent, enhanced dioxetane concns. are obsd. in MeOH and in nonprotic solvents with acid. The authors suggest a new mechanism that invokes a proton transfer from MeOH and HOBz to perepoxide (I) and zwitterion (II) intermediates.

IT **917-23-7**, meso-Tetraphenylporphyrin
RL: CAT (Catalyst use); USES (Uses)
(photosensitizer; formation of [2 + 2] products with added acid in reaction of singlet oxygen with trans-4-propenylanisole)

RN 917-23-7 CAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:639578 CAPLUS

DOCUMENT NUMBER: 134:29257
TITLE: Temperature effect on the epoxidation of olefins by an iron(iii) porphyrin complex and tert-alkyl hydroperoxides
AUTHOR(S): Nam, Wonwoo; Oh, So-Young; Lim, Mi Hee; Choi, Mee-Hwa; Han, So-Yeop; Jhon, Gil-Ja
CORPORATE SOURCE: Dep. Chem., Div. Mol. Life Sci., Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Chemical Communications (Cambridge) (2000), (18), 1787-1788
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:29257

AB An electron-deficient iron porphyrin complex catalyzes the epoxidn. of olefins by tert-alkyl hydroperoxides via radical-free **oxidn.** reactions in **aprotic** solvent; the epoxidn. reactions were markedly influenced by reaction temp. and high yields of epoxide products were obtained with retention of stereospecificity at low temp.

IT **156191-16-1**
RL: CAT (Catalyst use); USES (Uses)
(temp. effect on epoxidn. of olefins by iron porphyrin complex and tert-alkyl hydroperoxides)

RN 156191-16-1 CAPLUS
CN Iron(5+), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis[2,3,5,6-tetrafluoro-N,N,N-trimethylbenzenaminiumato]](2-)]-, (SP-4-1)-, salt with trifluoromethanesulfonic acid (1:5) (9CI) (CA INDEX NAME)

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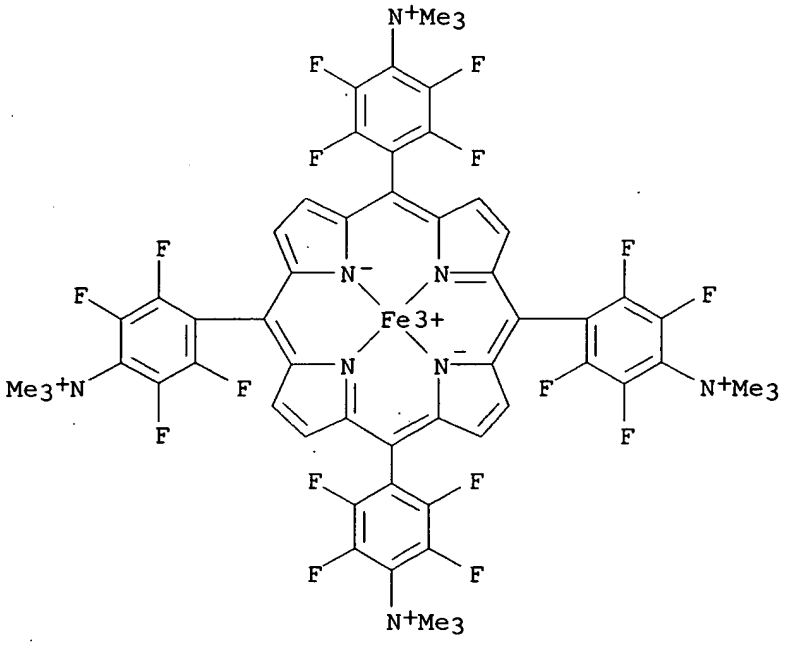
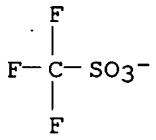
CRN 156191-15-0
CMF C56 H44 F16 Fe N8
CCI CCS



CM 2

CRN 37181-39-8
CMF C F3 O3 S



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:346510 CAPLUS
DOCUMENT NUMBER: 131:166940
TITLE: Biomimetic Alkane Hydroxylations by an Iron(III) Porphyrin Complex with H2O2 and by a High-Valent Iron(IV) Oxo Porphyrin Cation Radical Complex
AUTHOR(S): Nam, Wonwoo; Goh, Yeong Mee; Lee, Yoon Jung; Lim, Mi Hee; Kim, Cheal
CORPORATE SOURCE: Department of Chemistry and Center for Cell Signaling Research, Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Inorganic Chemistry (1999), 38(13), 3238-3240
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Iron(III) porphyrin complexes have been used as model compds. to mimic the chem. of cytochrome P 450 enzymes that are capable of catalyzing a wide range of **oxidn.** reactions, including the remarkably difficult hydroxylation of relatively unreactive C-H bonds of alkanes. Previous studies for iron-(III) porphyrin complex-catalyzed alkane hydroxylation reactions have been conducted extensively with oxidants such as PhIO, KHSO5, NaOCl, ROOH, O2, and ozone. However, as far as we have been able to discern, radical-free (enzyme mimetic) hydroxylation of alkanes with a biol. important oxidant (i.e. H2O2) has been rarely obsd. in iron porphyrin-catalyzed oxygenation reactions. Moreover, although high-valent iron(IV) oxo porphyrin cation radical species have been generally proposed as a reactive intermediate responsible for the C-H bond activation in cytochrome P 450 enzymes and iron porphyrin systems, and the presence of a high-valent iron oxo intermediate has been detected during the catalytic hydroxylation of ethylbenzene by ozone, direct hydroxylation reactions by "isolated" high-valent iron(IV) oxo porphyrin cation radical complexes have been rarely reported. In this note we report that an electronegatively-substituted iron porphyrin complex efficiently catalyzes the hydroxylation of alkanes by H2O2 via radical-free **oxidn.** reactions in **aprotic** solvent (i.e. CH3CN) and that an "isolated" high-valent iron(IV) oxo porphyrin cation radical intermediate of the iron porphyrin complex is capable of activating C-H bonds of alkanes to give oxygenated products efficiently even at low temp. We also present strong evidence that the hydroxylating intermediate generated in the catalytic H2O2 reaction is the high-valent iron-(IV) oxo porphyrin cation radical species.

IT **156191-15-0 215508-61-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(biomimetic alkane hydroxylation using iron(III) porphyrin complex with H2O2 and high-valent iron(IV) oxo porphyrin cation radical complex)

RN 156191-15-0 CAPLUS

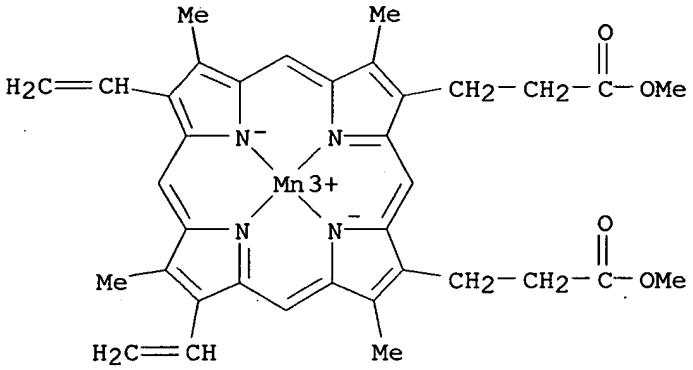
CN Iron(5+), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis[2,3,5,6-tetrafluoro-N,N,N-trimethylbenzenaminiumato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

L6 ANSWER 9 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:263966 CAPLUS
DOCUMENT NUMBER: 131:10757
TITLE: Reduction of Manganese(III) Protoporphyrin IX Dimethyl Ester Studied by Electrochemistry and Surface-Enhanced Raman Scattering Spectroscopy
AUTHOR(S): Chen, Shi-Ping; Williams, Anthony; Ejeh, David; Hambright, Peter; Hosten, Charles M.
CORPORATE SOURCE: Howard University, Washington, DC, 20059, USA
SOURCE: Langmuir (1999), 15(11), 3998-4004
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reductive electrochem. of manganese(III) protoporphyrin IX di-Me ester, MnIII(PPDME), in an **aprotic** solvent was studied using cyclic voltammetry, surface-enhanced Raman scattering spectroscopy (SERS), and thin layer potential dependent UV/visible absorption spectroscopy. Good quality SERS spectra are reported for an electrochem. roughened silver electrode in contact with Mn(PPDME) dissolved in acetonitrile. A reversible 1-electron redn. was obsd. at .apprx.-0.44 V/SCE in the cyclic voltammetric scans on silver, gold, and platinum electrodes. In thin layer UV/visible spectroelectrochem., the Soret band at 473 nm at 0.0 V undergoes a 36 nm blue shift to 437 nm when the electrode potential was stepped to -0.5 V. Resonance Raman and SERS spectral frequencies of Mn(PPDME) are assigned and tabulated. The shift of the Soret band along with the downshift in the .nu.4 **oxidn**. state marker band from 1373 to 1360 cm-1 in the SERS spectra identify the process occurring at .apprx.-0.5 V to be the redn. of the porphyrin central metal ion from the MnIII to MnII state. Core sizes for MnIII(PPDME) and MnII(PPDME) adsorbed on an anodized silver electrode surface are 1.993 and 2.072 .ANG., resp. Both the MnII and MnIII complexes are adsorbed as high spin, five-coordinate species. From relative intensities of the SERS bands, the orientation of Mn(PPDME) adsorbed onto the silver electrode surface probably is face-on.

IT **47856-39-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(electrochem. redn. in acetonitrile studied by cyclic voltammetry on silver or gold or platinum electrodes and by surface-enhanced Raman scattering spectroscopy and potential-dependent UV/visible spectroscopy)

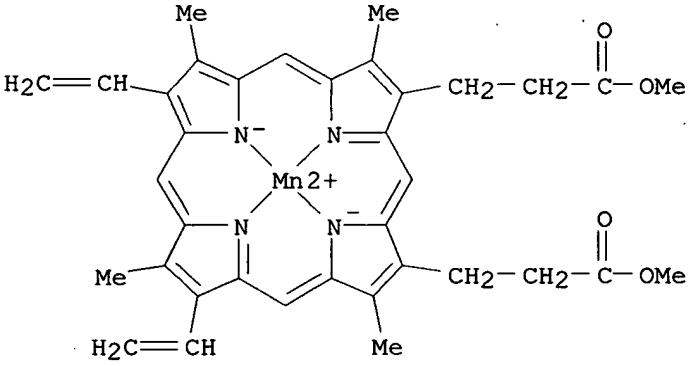
RN 47856-39-3 CAPLUS
CN Manganese(1+), [dimethyl 7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **30789-56-1**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(electrochem. reductive formation in acetonitrile studied by cyclic voltammetry on silver or gold or platinum electrodes and by surface-enhanced Raman scattering spectroscopy and potential-dependent UV/visible spectroscopy)

RN 30789-56-1 CAPLUS

CN Manganese, [dimethyl 7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

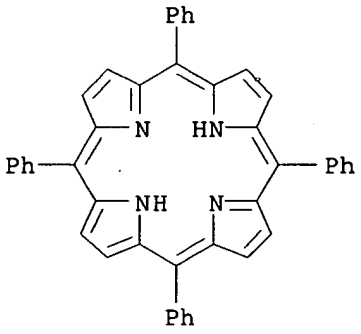
L6 ANSWER 10 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:499531 CAPLUS
DOCUMENT NUMBER: 129:230362
TITLE: Primary and Secondary Isotope Effects in the Photooxidation of 2,5-Dimethyl-2,4-hexadiene. Elucidation of the Reaction Energy Profile
AUTHOR(S): Vassilikogiannakis, Georgios; Stratakis, Manolis; Orfanopoulos, Michael
CORPORATE SOURCE: Department of Chemistry, University of Crete, Iraklion, 71409, Greece

SOURCE: Journal of Organic Chemistry (1998), 63(18), 6390-6393
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:230362

AB The mechanism of the ene, [2 + 2], and methanol-trapping pathways in the sensitized photooxygenation of the 2,5-dimethyl-2,4-hexadiene are discussed. The formation of a perepoxide is a common intermediate in the first step for all reaction paths. Dioxetane and methoxy adducts are probably formed via an open biradicaloid zwitterionic intermediate, which is produced by rearrangement of the perepoxide in a faster step. The perepoxide is formed reversibly in a fast step compared to the competing ene step. Although the ene pathway is energetically unfavorable , it becomes predominant in **aprotic** solvents, due to the significant collapse of the zwitterionic intermediate to starting materials.

IT **917-23-7**, Tetraphenylporphine
RL: CAT (Catalyst use); USES (Uses)
(sensitizer; primary and secondary isotope effects in photooxidn. of 2,5-dimethyl-2,4-hexadiene. elucidation of reaction energy profile)

RN 917-23-7 CAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 45 CAPLUS COPYRIGHT 2003 ACS

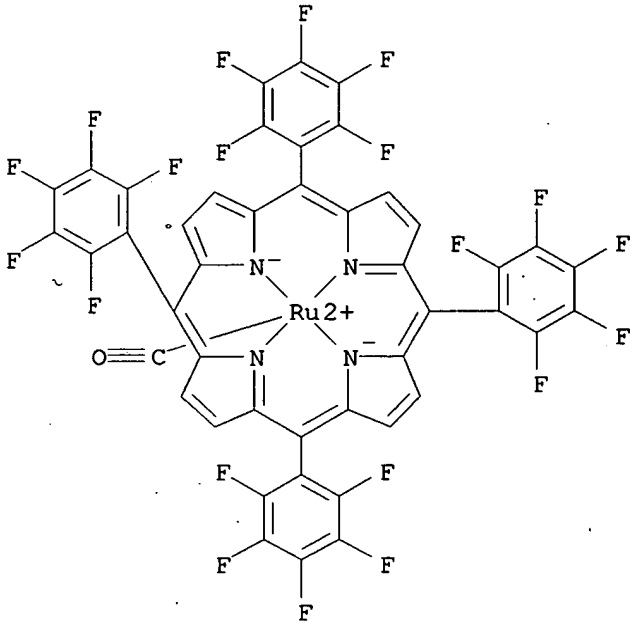
ACCESSION NUMBER: 1998:93389 CAPLUS
DOCUMENT NUMBER: 128:180083
TITLE: Rapid catalytic oxygenation of hydrocarbons with perhalogenated ruthenium porphyrin complexes
AUTHOR(S): Groves, John T.; Shalyaev, Kirill V.; Bonchio, Marcella; Carofiglio, Tommaso
CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA
SOURCE: Studies in Surface Science and Catalysis (1997), 110(3rd World Congress on Oxidation Catalysis, 1997), 865-872
CODEN: SSCTDM; ISSN: 0167-2991
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Conference proceedings. Perhalogenated ruthenium porphyrins were found to be efficient catalysts for the oxygenation of hydrocarbons including secondary alkanes and benzene in the presence of 2,6-dichloropyridine N-oxide under mild conditions in **aprotic** media. Up to 15,000 turnovers and rates of 800 TO/min were obtained. A mechanism where Ru(III) - Ru(V) intermediates play an important role is proposed and discussed.

IT **171899-61-9 185009-67-0**
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(rapid catalytic oxygenation of hydrocarbons with perhalogenated ruthenium porphyrin complexes)

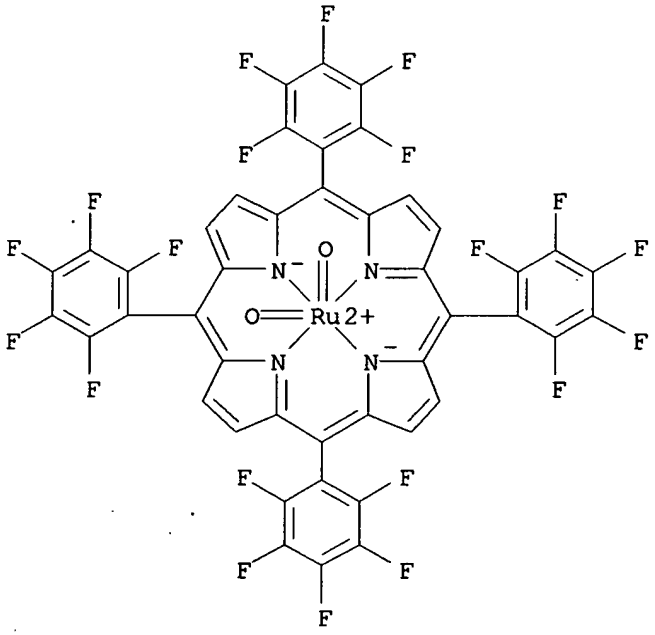
RN 171899-61-9 CAPLUS

CN Ruthenium, carbonyl[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-31)-(9CI) (CA INDEX NAME)



RN 185009-67-0 CAPLUS

CN Ruthenium, dioxo[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (OC-6-12)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:433608 CAPLUS
DOCUMENT NUMBER: 127:127858
TITLE: Reactivity toward Dioxygen of Dicobalt Face-to-Face Diporphyrins in **Aprotic** Media. Experimental and Theoretical Aspects. Possible Mechanistic Implication in the Reduction of Dioxygen
AUTHOR(S): Le Mest, Yves; Inisan, Claude; Laouenan, Andre; L'Her, Maurice; Talarmin, Jean; El Khalifa, Moulay; Saillard, Jean-Yves
CORPORATE SOURCE: Laboratoire de Chimie Electrochimie Moleculaires et Chimie Analytique, Universite de Bretagne Occidentale, Brest, 29285, Fr.
SOURCE: Journal of the American Chemical Society (1997), 119(26), 6095-6106
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

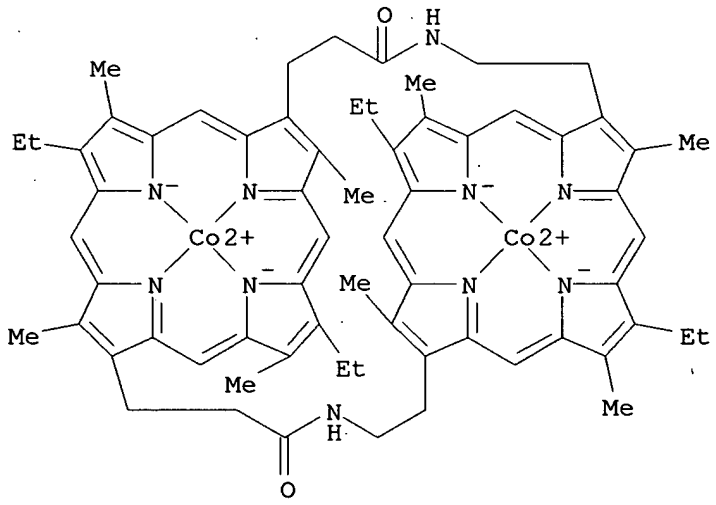
AB The reactivity toward dioxygen of two series of dicobalt cofacial diporphyrins in soln. in an **aprotic** solvent is described. Some of these compds. are efficient electrocatalysts for the four-electron redn. of dioxygen when adsorbed on a graphite electrode immersed in aq. acid. Their electrochem. and spectroscopic (UV-visible, EPR) behavior in soln. shows that, contrary to what is obsd. with cobalt monomers, the neutral [PCoIICoIIP] (1) (P stands for a porphyrin ring) form does not react with dioxygen. Uniquely the 1- and two-electron-oxidized forms of the dimer, [PCoII.cntdot.CoIIP]+ (1+) and [PCoII---CoIIP]2+ (12+), resp., reversibly bind dioxygen, giving two complexes, 2 and 3, at room temp. and in the absence of a good axial ligand. The stability consts. of the two

O2 complexes were measured spectrophotometrically and/or electrochem., and prove to be remarkably high. As a whole, the present O2 binding processes appear unprecedented as basically different in many respects from the process classically described in the case of cobalt monomers. EHMO calcns., based on the crystal structure of the Co2FTF4 dimer in its uncomplexed form (Co-Co distance 3.42 .ANG.), show that, in the absence of very important deformations of its structure, the only possible geometry for the O2 complex of the two-electron-oxidized deriv. [PCo-O2-CoP]2+ (3) is the .mu.-.eta.2:.eta.2-peroxo structure. The calcd. corresponding electronic diagram affords a rationale for most of the exptl. obsd. properties. Specifically, the O2 complex of the 1-electron-oxidized form [PCo-O2.bul.-CoP]+ (2), the reduced form of complex 3, should be considered as a species in which the O2 moiety is further reduced, at least partially, as compared to its peroxo state in 3, i.e., consequently in an **oxidn.** state intermediate between peroxo (-1) and oxo (-2). Preliminary results indicate that this species reacts with one proton, while the two-electron-oxidized O2 complex 3 is resistant to protonation. The possible implications of these specific properties of the dicobalt dimers in the four-electron redn. mechanism of O2 are discussed, and structural and mechanistic similarities with bioinorg. dinuclear sites appear significant.

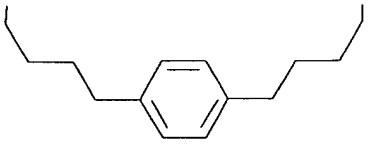
IT **71253-22-0 71253-24-2 74436-37-6 74452-74-7 88563-09-1 94250-18-7**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(electrochem. **oxidn.** in benzonitrile under oxygen: reactivity toward dioxygen of dicobalt face-to-face diporphyrins in **aprotic** media and exptl. and theor. aspects and possible mechanistic implication in redn. of dioxygen)

RN 71253-22-0 CAPLUS

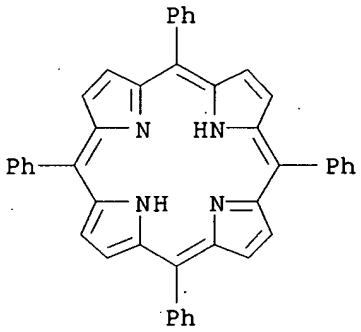
CN Cobalt, [.mu.-[16,35,45,53-tetraethyl-5,6,8,9,23,24,27,28-octahydro-3,17,22,36,40,46,52,56-octamethyl-43H,50H-15,18:34,37-diimino-13,10:32,29-dimetheno-2,30:11,21-bis(metheno[2,5]-endo-pyrrolometheno)dipyrrolo[2,3-n:2',3'-f1][1,6,18,24]tetraazacyclohexatriacontine-7,25(4H,26H)-dionato(4-)-.kappa.N1,.kappa.N31,.kappa.N39,.kappa.N43:.kappa.N12,.kappa.N20,.kappa.N50,.kappa.N55]]di- (9CI) (CA INDEX NAME)



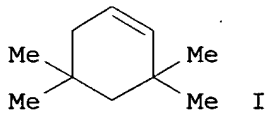
PAGE 2-A



IT **917-23-7**, Tetraphenylporphyrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with rhodium chloride)
RN 917-23-7 CAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 14 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:718164 CAPLUS
DOCUMENT NUMBER: 123:339177
TITLE: Tetra(2,6-dichlorophenyl)porphyrin - a superior sensitizer for the singlet-oxygen ene reaction (Schenck Reaction)
AUTHOR(S): Quast, Helmut; Dietz, Thomas; Witzel, Alexander
CORPORATE SOURCE: Inst. Organische Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany
SOURCE: Liebigs Annalen (1995), (8), 1495-501
CODEN: LANAEM; ISSN: 0947-3440
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

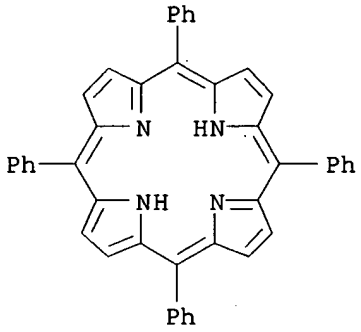
AB The very useful singlet-oxygen ene reaction of reluctant cycloalkenes (e.g. I) and, in particular, mono(allyl hydroperoxides) , is handicapped by the instability of the sensitizer TPP. A comparative study of TPP, TPFPP,

and TDCPP in the singlet-oxygen ene reaction of these alkenes shows that (1) the persistence increases in the order TPP < TPFPP > TDCPP, rendering TDCPP the sensitizer of choice for the generation of singlet-oxygen in non-polar solvents, (2) the persistence of the tetraarylporphyrins decreases in the presence of an alkene, (3) this decrease strongly depends on the nature of the alkene, being most pronounced in the case of cyclohexene. These results are interpreted in terms of unknown substrate-derived species which induce oxidative destruction of the tetraarylporphyrins. Alternatively, abstraction of allylic hydrogen atoms from the alkenes by the excited sensitizers may give rise to the obsd. substrate-dependent photobleaching. Because the single-oxygen ene reaction is the key step of a 1,2-carbonyl transposition with concomitant dehydrogenation, the scope and usefulness of this sequence are distinctly improved.

IT **917-23-7**, 5,10,15,20-Tetraphenylporphyrin **25440-14-6**, 5,10,15,20-Tetrakis(pentafluorophenyl)porphyrin **37083-37-7**, 5,10,15,20-Tetrakis(2,6-dichlorophenyl)porphyrin
RL: NUU (Other use, unclassified); USES (Uses)
(sensitizer of choice for generation of singlet oxygen in **aprotic** org. solvents)

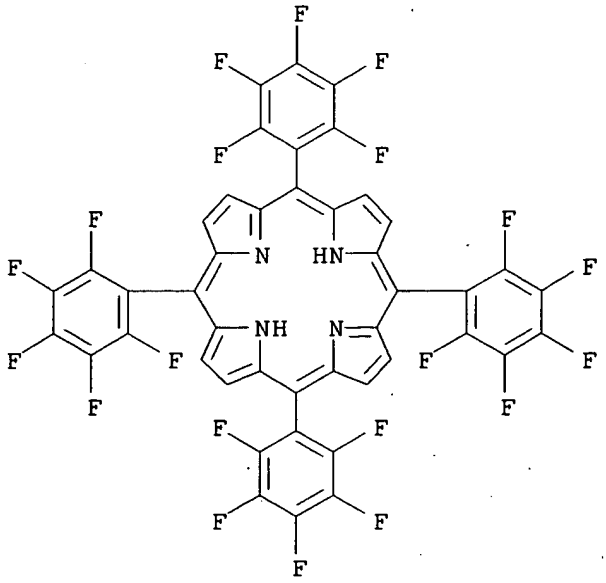
RN 917-23-7 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

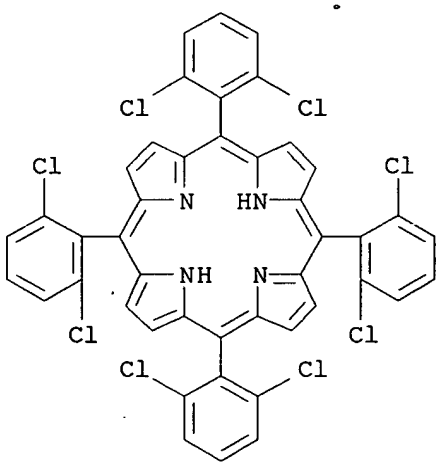


RN 25440-14-6 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)



RN 37083-37-7 CAPLUS
CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 15 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:550750 CAPLUS
DOCUMENT NUMBER: 121:150750
TITLE: pH-Dependent One- and Two-Electron **Oxidation** of 3,5-Dicarbethoxy-2,6-dimethyl-4-ethyl-1,4-dihydropyridine Catalyzed by Horseradish Peroxidase
AUTHOR(S): Sugiyama, Katsumi; Correia, Maria A.; Thummel, Kenneth E.; Nagata, Kiyoshi; Darbyshire, John F.; Osawa, Yoichi; Gillette, James R.
CORPORATE SOURCE: Laboratory of Chemical Pharmacology, National Heart

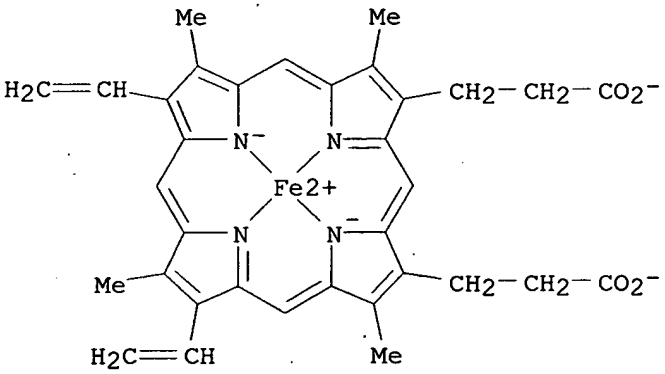
Lung and Blood Institute, Bethesda, MD, 20892, USA
SOURCE: Chemical Research in Toxicology (1994), 7(5), 633-42
CODEN: CRTOEC; ISSN: 0893-228X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The porphyrinogenic agent 3,5-dicarbethoxy-2,6-dimethyl-4-ethyl-1,4-dihydropyridine (DDEP) is known to inactivate hepatic cytochrome P 450 (P 450) enzymes 2C11, 2C6, and 3A1 (1987) by different mechanisms. The authors have found that DDEP inactivates horseradish peroxidase (HRP) pretreated with hydrogen peroxide. In this system, DDEP was oxidized predominately to 3,5-dicarbethoxy-2,6-dimethyl-4-ethylpyridine (EDP) under weakly acidic conditions and predominately to 3,5-dicarbethoxy-2,6-dimethylpyridine (DP) under basic conditions. The loss of heme and the formation of altered heme products were also pH-dependent and were correlated with the formation of DP and the inactivation of HRP. Thus, the inactivation of HRP appears to depend on the formation of an Et radical, which presumably reacts with the heme in the active site of the enzyme. Similar product ratios were obtained for the **oxidn.** of DDEP by K3Fe(CN)6, indicating that product ratios of DP over EDP are mainly detd. by the pH of buffer. These results, in addn. to semiempirical calcns. (AM1) for the **oxidn.** of DDEP in the gas phase, are consistent with the idea that the inhibitor undergoes a single-electron **oxidn.** to form the DDEP radical cation, the fate of which depends on the environment of the active site of the enzyme. The proposed formation of a radical cation by the abstraction of an electron from nitrogen is consistent with the finding of low intramol. isotope effects of the metab. of 3,5-dicarbethoxy-2,6-dimethyl-[4-2H,4-1H]-1,4-dihydropyridine by P 450 2C11 and 3A4. Under basic or **aprotic** conditions, the radical dissocs. to form DP and the Et radical, which reacts with the heme, thereby inactivating the enzyme. Under acidic or polar conditions, the radical undergoes an addnl. one-electron **oxidn.** to form EDP. Since DP is the predominant product in P 450 2C6- and 2C11-catalyzed reactions (1989), these findings suggest that the active sites of P 450 2C11 and 2C6 are lipophilic and/or basic. By contrast, P 450 3A1 converts DDEP predominately to EDP, suggesting that the active site of this enzyme is polar and/or acidic.

IT **14875-96-8,** Heme
RL: BIOL (Biological study)
(dicarbethoxydimethylethyldihydropyridine horseradish peroxidase-catalyzed **oxidn.** in relation to)

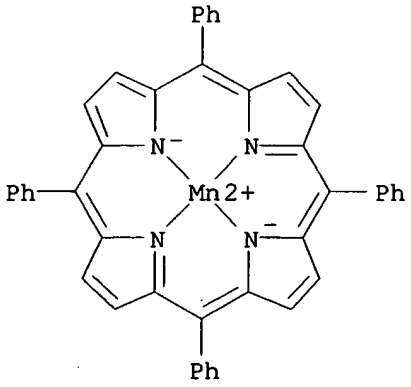
RN 14875-96-8 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)

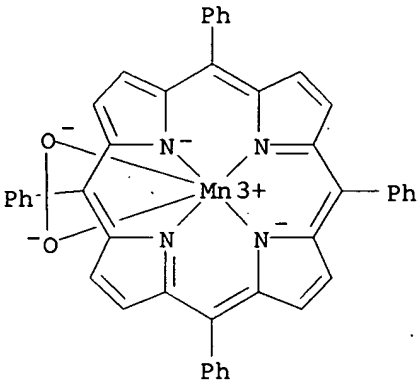


●2 H^+

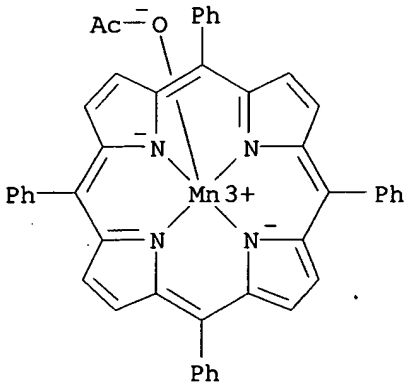
L6 ANSWER 16 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:494337 CAPLUS
DOCUMENT NUMBER: 121:94337
TITLE: Interaction of Mn(III) tetraphenylporphyrin with superoxide; the reaction mechanism and evidence for a peroxo complex
AUTHOR(S): Lang, Kamil; Vondrak, Jiri; Wagnerova, Dana M.
CORPORATE SOURCE: Inst. Inorg. Chem., Acad. Sci. Czech Republic, Prague, 160 00, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (1994), 59(5), 1059-65
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cathodic 1-electron redn. of Mn(III)TPP and O2 in an **aprotic** solvent yields Mn(II)TPP and the superoxide anion radical O2-. The Mn(II)TPP and O2- react in soln. to the side-on peroxo complex Mn(III)TPP-O22-, which is oxidized at the electrode at a peak potential of Epa = 0.40 V vs. normal H electrode (k .apprxeq. 104 dm3 mol-1 s-1). The rate-detg. step of the overall 2-electron **oxidn.** is the transfer of the 1st electron coupled with a structure rearrangement of the peroxo complex to a superoxo complex.
IT **31004-82-7**, Manganese(II) tetraphenylporphyrin
RL: PRP (Properties)
(interaction of electrogenerated, with electrogenerated superoxide in **aprotic** solvent)
RN 31004-82-7 CAPLUS
CN Manganese, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT **106266-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**oxidn.** of, electrochem.)
RN 106266-46-0 CAPLUS
CN Manganate(1-), peroxy[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]- (9CI) (CA INDEX NAME)



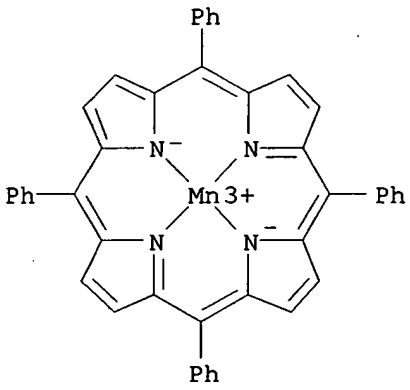
IT **58356-65-3**
RL: PRP (Properties)
(redn. of oxygen and, in **aprotic** solvent, interaction of manganese tetraphenylporphyrin and superoxide in relation to)
RN 58356-65-3 CAPLUS
CN Manganese, (acetato-.kappa.O)[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



L6 ANSWER 17 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:435209 CAPLUS
DOCUMENT NUMBER: 121:35209
TITLE: Development of the Copper-Catalyzed Olefin Aziridination Reaction
AUTHOR(S): Evans, David A.; Bilodeau, Mark T.; Faul, Margaret M.
CORPORATE SOURCE: Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (1994), 116(7), 2742-53
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

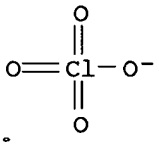
AB Sol. Cu(I) and Cu(II) triflate and perchlorate salts are efficient catalysts for the aziridination of olefins employing (N-(p-tolylsulfonyl)imino)phenyliodinane, PhI:NTs, as the nitrene precursor. Electron-rich as well as electron-deficient olefins undergo aziridination with this reagent in 55-95% yields, at temps. ranging from -20 .degree.C to +25 .degree.C. The catalyzed nitrogen atom-transfer reaction to enol silanes and silylketene acetals has also been developed to provide facile syntheses of .alpha.-amino ketones. Other metal complexes were found to be less effective at catalyzing the reaction, while PhI:NTs proved to be superior to other imido group donors as the nitrene precursor. Reaction rates and yields are enhanced in polar **aprotic** solvents such as MeCN and MeNO2. Reaction stereospecificity in the aziridination of cis and trans disubstituted olefins was evaluated and found to be both catalyst and substrate dependent. Intermol. competition expts. between pairs of mono- and disubstituted olefins indicate that the olefin selectivity profile for the reaction is independent of the **oxidn**. state of the copper catalyst employed. It is concluded that these reactions are proceeding through the 2+ catalyst **oxidn**. state under the conditions employed in this study.

IT **16456-81-8 32195-55-4 79408-54-1**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for aziridination of olefins by [(p-tolylsulfonyl)imino]phenyliodinane)
RN 16456-81-8 CAPLUS
CN Iron, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



CM 2

CRN 14797-73-0
CMF Cl O4



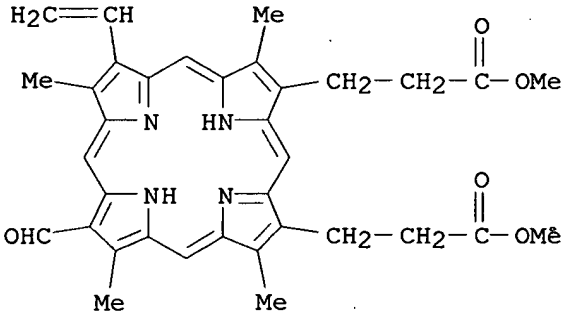
L6 ANSWER 18 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:100737 CAPLUS
DOCUMENT NUMBER: 120:100737
TITLE: Photodegradation of protoporphyrin dimethyl ester in solution and in organized environments
AUTHOR(S): Wessels, J. M.; Sroka, R.; Heil, P.; Seidlitz, H. K.
CORPORATE SOURCE: Inst. Biophys. Strahlenforsch., GSF-Forschungszent. Umwelt Gesundheit, Neuherberg, D-85764, Germany
SOURCE: International Journal of Radiation Biology (1993), 64(5), 475-84
CODEN: IJRBE7; ISSN: 0955-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The degrdn. of sensitizers used in photodynamic therapy (PDT) involves photooxidn. either by mol. oxygen or by oxygen intermediates which leads to hydroxy aldehyde and formyl products or to ring opening. The authors' investigations focused on the spectroscopic changes which protoporphyrin-dimethyl ester (PP) exhibits upon irradn. As the microenvironment strongly influences the effects, the authors used an **aprotic** org. solvent, L-.alpha.-dioleoylphosphatidylcholine (DOPC) liposomes and isogenic fibrosarcoma cells (SSKII) as carriers for PP. Hydroxy aldehyde product isomers developed a new absorption band centered around 670 nm and a new emission band at 676 nm. These characteristics can be used to discriminate them from formyl products and intact PP. In org. solvents, the formation of the hydroxy aldehyde products predominated. In DOPC liposomes and cells, the hydroxy aldehyde yield drops and photooxidn. results in attack of the macrocycle. Time-resolved

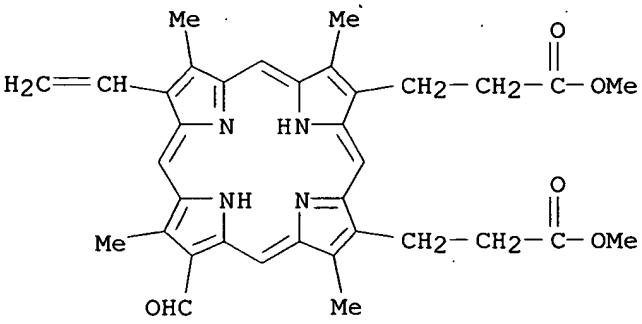
fluorescence spectroscopy of monomeric PP in an org. solvent gives a monoexponential decay time of 10.1 ns. Upon irradn. a second component with a decay time of 4.9 ns, resulting from the hydroxy aldehyde product, was detected. In liposomes and cells, the monomeric decay time was significantly longer (15 ns) due to the altered microenvironment. Addnl., the authors obsd. in liposomes and in cells a small contribution of a short component (1 ns) which is attributed to an aggregated sensitizer species. In irradiated cells, the aggregated fraction doubled, indicating a change in the microenvironment caused by the photodynamic action of the sensitizer.

IT **10200-04-1 13187-15-0 15341-25-0**
RL: FORM (Formation, nonpreparative)
(formation of, during photodegrdn. of protoporphyrin di-Me ester in soln. and in organized environments)

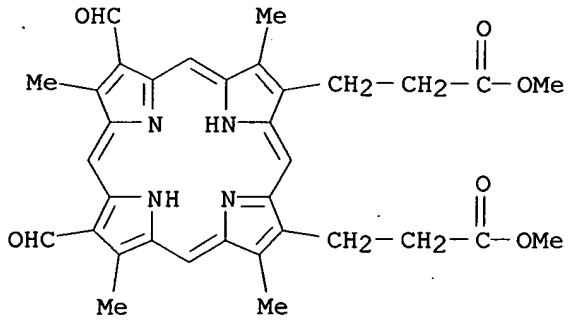
RN 10200-04-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7-ethenyl-12-formyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



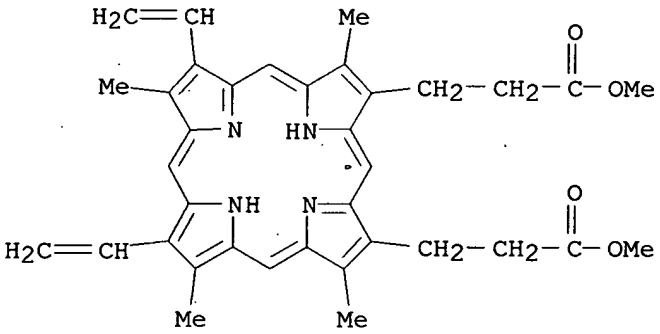
RN 13187-15-0 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 8-ethenyl-13-formyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 15341-25-0 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diformyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



IT **5522-66-7**, Protoporphyrin dimethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(photodegrdn. of, in soln. and in organized environments)
RN 5522-66-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



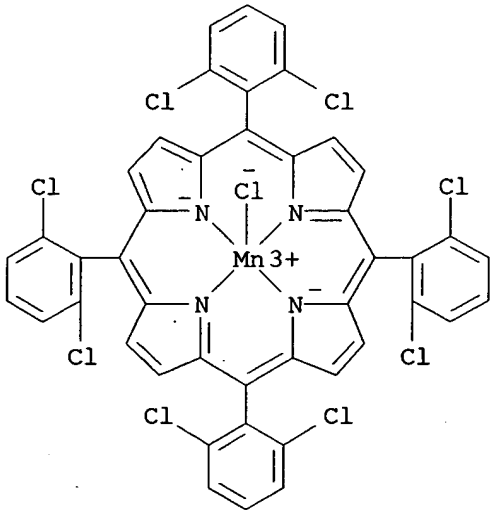
L6 ANSWER 19 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:190966 CAPLUS
DOCUMENT NUMBER: 118:190966
TITLE: Reevaluation of the significance of oxygen-18 incorporation in metal complex-catalyzed oxygenation reactions carried out in the presence of oxygen-18-labeled water (H218O)
AUTHOR(S): Nam, Wonwoo; Valentine, Joan Selverstone
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024, USA
SOURCE: Journal of the American Chemical Society (1993), 115(5), 1772-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The extent of 18O incorporation into the products of metal complex-catalyzed oxygenations of org. compds. was measured when H218O was added to the reaction mixt. The oxidants studied were hydrogen peroxide, tert-Bu hydroperoxide, m-chloroperbenzoic acid (MCPBA), and iodosylbenzene, and the reactions were carried out in org. solvents. In reactions of hydrogen peroxide, tert-Bu hydroperoxide, and MCPBA, no or at

most a small amt. of 18O was incorporated into the products in either olefin epoxidn. or alkane hydroxylation reactions catalyzed by (meso-tetrakis(2,6-dichlorophenyl)porphinato)iron(III) chloride [Fe(TDCPP)Cl], (meso-tetrakis(2,6-dichlorophenyl)porphinato)manganese(III) chloride [Mn(TDCPP)Cl] with imidazole added, iron(II) cyclam (cyclam = 1,4,8,11-tetraazacyclotetradecane), manganese(II) cyclam, and nickel(II) cyclam. Assuming that high-valent metal oxo intermediates are generated in all of the reactions of iron and manganese porphyrin complexes with the oxidants PhIO, H2O2, tert-Bu hydroperoxide, and MCPBA, the high-valent iron oxo and manganese oxo intermediates do not exchange or slowly exchange with labeled H218O during the course of these catalytic oxygenation reactions. Several different iron(III) and manganese(III) porphyrin complexes such as Fe(TDCPP)Cl, (meso-tetraphenylporphinato)iron(III) chloride [Fe(TPP)Cl], (meso-tetramesitylporphinato)iron(III) chloride [Fe(TMP)Cl], and Mn(TDCPP)Cl were used to catalyze cyclohexene epoxidn. by MCPBA at -78.degree. in the presence of H218O. The epoxide obtained in the epoxidn. of cyclohexene catalyzed by Fe(TDCPP)Cl, Fe(TPP)Cl, Fe(TMP)Cl, and Mn(TDCPP)Cl contained 0%, 4%, 22%, and 0% 18O, resp. By contrast, in the iodosylbenzene reactions, oxygen from labeled H218O was fully incorporated into products in **aprotic** and protic solvents in olefin epoxidn. and alkane hydroxylation reactions catalyzed by either iron(III) porphyrin, manganese(III) porphyrin, or metallocyclam (M = Fe, Mn, Ni) complexes. Labeled oxygen from H218O was also fully incorporated into cyclohexene oxide in the epoxidn. of cyclohexene catalyzed by a zinc complex which is not able to form a high-valent zinc oxo species as an intermediate. Thus, in the case of iodosylbenzene, the mechanism for oxygen exchange does not involve metal oxo intermediates and the observation of incorporation of labeled oxygen from H218O into products does not provide evidence for the intermediacy of metal oxo complexes in iodosylbenzene reactions. In the case of oxidants other than iodosylbenzene, the results also suggest that reactions of high-valent metal oxo complexes with org. substrates in catalytic oxygenation reactions are often comparable in rate to or faster than the reactions with isotopically labeled water that lead to oxygen exchange.

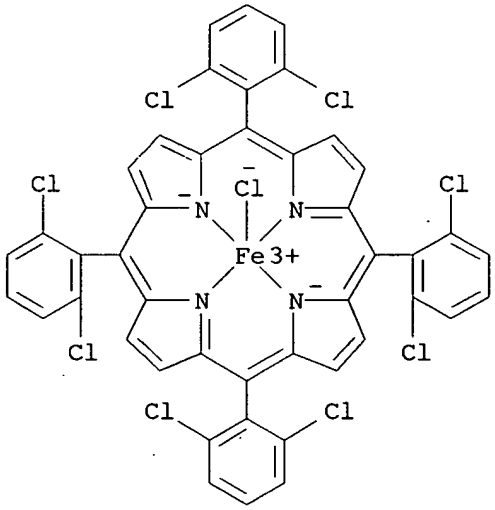
IT **91463-17-1**
RL: CAT (Catalyst use); USES (Uses)
(catalysts from imidazole and, for **oxidn**. of org. compds., mechanism with)

RN 91463-17-1 CAPLUS

CN Manganese, chloro[5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-(9CI) (CA INDEX NAME)



IT **91042-27-2**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for **oxidn.** of org. compds., mechanism with)
RN 91042-27-2 CAPLUS
CN Iron, chloro[5,10,15,20-tetrakis(2,6-dichlorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

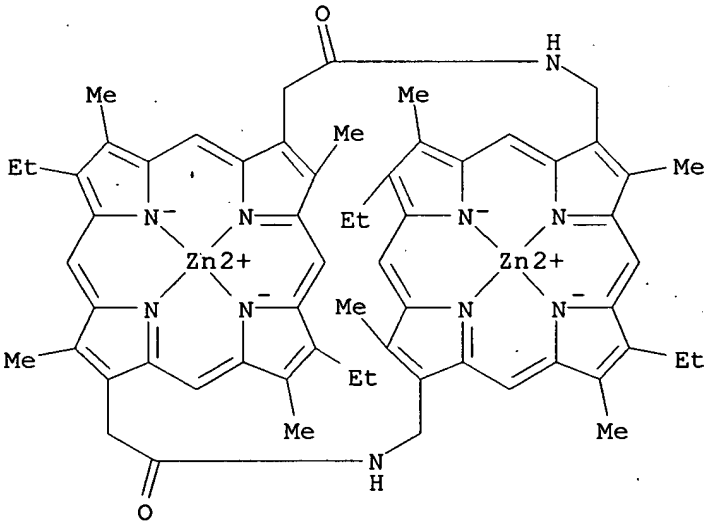


L6 ANSWER 20 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:70327 CAPLUS
DOCUMENT NUMBER: 116:70327
TITLE: Enhanced electronic delocalization in face-to-face diporphyrins: implication in the unique reactivity of the cobalt derivatives towards dioxygen and in the 4-electron reduction mechanism of oxygen

AUTHOR(S): Le Mest, Y.; L'Her, M.; Collman, J. P.
CORPORATE SOURCE: Univ. Bretagne Occident., Brest, 29287, Fr.
SOURCE: Studies in Surface Science and Catalysis (1991), 66(Dioxygen Act. Homogeneous Catal. Oxid.), 229-35
CODEN: SSCTDM; ISSN: 0167-2991
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The electrochem. and spectroscopic (UV-visible, EPR) properties of two series of dimeric cofacial porphyrins were studied in **aprotic** media under an inert atm., and in the presence of dioxygen. The existence of a cofacial effect created by the geometry of these dimers induces a new mechanistic pathway for the O2 fixation by the dicobalt derivs., in which, not only the electrons of the cobalt(II) but also those of the porphyrin rings are involved. Two kinds of complexes are obtained: a .mu.-superoxo and a .nu.-peroxo deriv. The availability of the electrons of the rings could be a clue to the comprehension of the mechanism by which these compds. promote the 4-electron redn. of dioxygen.

IT **90818-97-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**Oxidn.** of, electrochem., on platinum in benzonitrile)
RN 90818-97-6 CAPLUS
CN Zinc, [.mu.-[14,31,41,49-tetraethyl-4,5,23,24-tetrahydro-3,15,20,32,36,42,48,52-octamethyl-39H,46H-13,16:30,33-diimino-11,8:28,25-dimetheno-2,26:9,19-bis(metheno[2,5]-endo-pyrrolometheno)dipyrrolo[2,3-m:2',3'-c1][1,5,16,21]tetraazacyclodotriacontine-6,22(7H,21H)-dionato(4-)-N1,N27,N35,N39:N10,N18,N46,N51]]di- (9CI) (CA INDEX NAME)



IT **89906-36-5 96610-74-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(electrochem. prepn. and reaction of, with oxygen)
RN 89906-36-5 CAPLUS
CN Cobalt(1+), [.mu.-[14,31,41,49-tetraethyl-4,5,23,24-tetrahydro-3,15,20,32,36,42,48,52-octamethyl-39H,46H-13,16:30,33-diimino-11,8:28,25-dimetheno-2,26:9,19-bis(metheno[2,5]-endo-pyrrolometheno)dipyrrolo[2,3-m:2',3'-c1][1,5,16,21]tetraazacyclodotriacontine-6,22(7H,21H)-dionato(4-)-N1,N27,N35,N39:N10,N18,N46,N51]]di- (9CI) (CA INDEX NAME)

L6 ANSWER 21 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:41159 CAPLUS
DOCUMENT NUMBER: 116:41159
TITLE: Molecular recognition via base pairing: photoinduced electron transfer in hydrogen-bonded zinc porphyrin-benzoquinone conjugates
AUTHOR(S): Harriman, Anthony; Kubo, Yuji; Sessler, Jonathan L.
CORPORATE SOURCE: Cent. Fast Kinet. Res., Univ. Texas, Austin, TX, 78712, USA
SOURCE: Journal of the American Chemical Society (1992), 114(1), 388-90
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

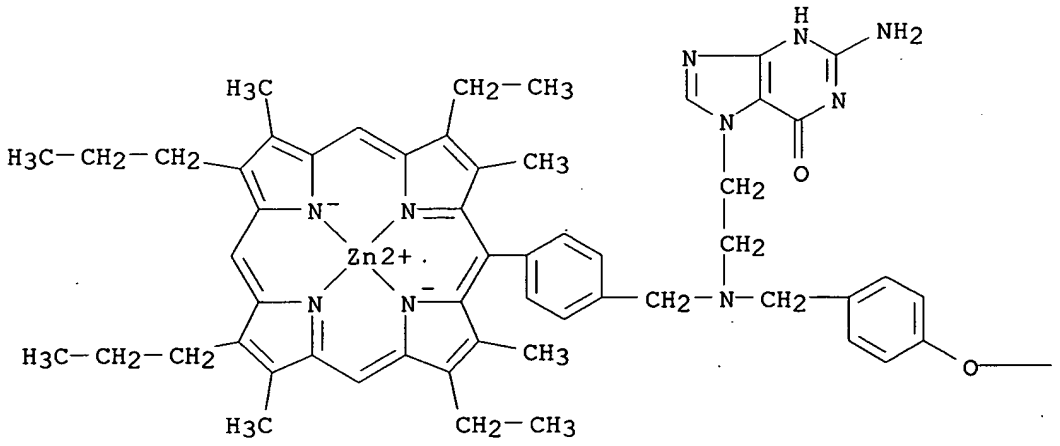
AB Cytosine and guanine derivs. covalently attached to redox-active porphyrin and quinone moieties resp. have been synthesized. The self-aggregation and photoinduced electron transfer properties of these putative noncovalent synthetic model systems are described. Specifically, mixing of the quinone-bearing cytosine I and the zinc porphyrin II functionalized with a guanine residue in **aprotic** solvents results in the formation of a hydrogen-bonded porphyrin-quinone conjugate. Upon illumination of the conjugate, electron transfer occurs from the porphyrin subunit to the adjacent quinone. The rate of electron transfer is (4.2 .+-. 0.7) .times. 108 s-1. Control expts., involving various systems with free or protected nucleic acid bases, served to show that the quinone function is mandatory for quenching to occur and that, in the absence of base-pairing, only bimol. quenching processes prevail. A binding const. for cytosine-guanine assocn. in CH2Cl2 of (1,290 .+-. 230) M-1 was obtained from fluorescence studies; this compares to a value of (3,100 .+-. 470) M-1 obtained by 1H NMR methods using a set of org. solubilized cytosine and guanine derivs.

IT **137895-26-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of)

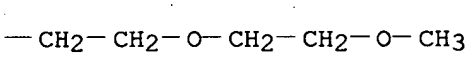
RN 137895-26-2 CAPLUS

CN 6H-Purin-6-one, 2-amino-7-[2-[[[4-(2,8-diethyl-3,7,12,18-tetramethyl-13,17-dipropyl-21H,23H-porphin-5-yl)phenyl]methyl][[4-[2-(2-methoxyethoxy)ethoxy]phenyl]methyl]amino]ethyl]-1,7-dihydro- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

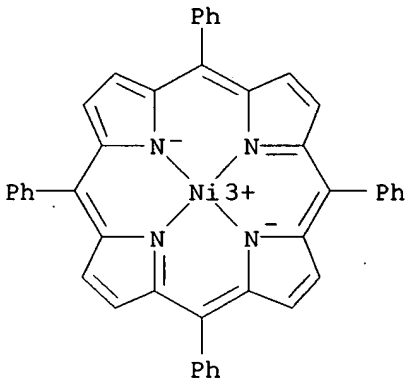


L6 ANSWER 22 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:237425 CAPLUS
DOCUMENT NUMBER: 114:237425
TITLE: One-electron **oxidation** of nickel porphyrins: effect of structure and medium on formation of nickel(III) porphyrin or nickel(II) porphyrin .pi.-radical cation
AUTHOR(S): Nahor, G. S.; Neta, P.; Hambright, P.; Robinson, L. R.
CORPORATE SOURCE: Chem. Kinet. Div., Natl. Inst. Stand. Technol., Gaithersburg, MD, 20899, USA
SOURCE: Journal of Physical Chemistry (1991), 95(11), 4415-18
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The **oxidn**. of several nickel(II) porphyrins by various radicals was studied by pulse radiolysis in different media (Cl2.bul.+ and Br2.bul.- in aq. systems, Br atoms in org. solvents, and peroxy radicals

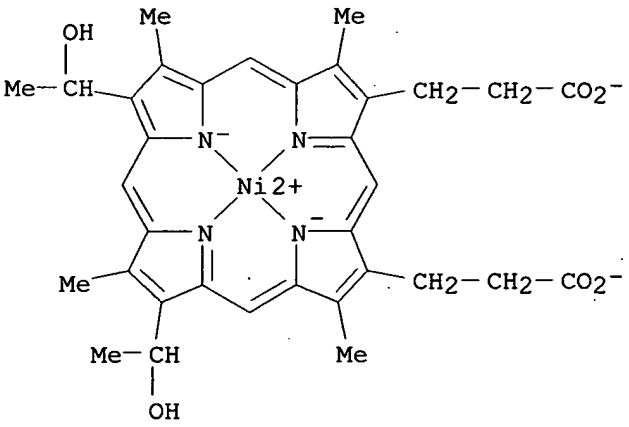
in org. and aq./org. systems). Photochem. **oxidn.** was also examd. in some cases. The absorption spectrum of the **oxidn.** product was monitored within several microseconds after the pulse. Two types of differential spectra were obsd., a broad absorption at 640-700 nm ascribed to the .pi.-radical cation, or a sharp absorption at 560-580 nm ascribed to nickel(III) porphyrin. NiIITPP (tetraphenylporphyrin) in several org. solvents, protic and **aprotic**, was oxidized to NiIIITPP. The addn. of 10% water as cosolvent or 0.1 M of electrolyte changed the route of **oxidn.** to give the radical cation NiIITPP.bul.+. On the other hand, NiIITSPP (tetrakis(4-sulfonatophenyl)porphyrin), which has 4 neg. charges, was oxidized on the porphyrin ligand by all the radicals examd., in water and in several org. solvents. NiII bis(N-methyl-4-pyridyl)diphenylporphyrin, with a charge of +2, and NiII tris(4-sulfonatophenyl)(N-methyl-4-pyridyl)porphyrin, with an overall charge of -2, were oxidized on the ligand in aq. soln., but on the metal in org. solvents. It is concluded that most radicals react with NiIIP by an inner-sphere mechanism to bind onto the metal and give the NiIIIP form. When the porphyrin is sufficiently charged to repel the axially bound anion, and/or when the medium enhances the sepn. of this anion from the metal, the result is **oxidn.** of the porphyrin .pi.-system. In all cases, however, the one-electron-**oxidn.** products, whether NiIIP.bul.+ or NiIIIP, decay to yield two-electron ring **oxidn.** products.

IT **29484-62-6P 133815-76-6P 133815-77-7P 133815-78-8P 133815-79-9P 133815-80-2P 133815-81-3P**
RL: PREP (Preparation)
(formation and optical absorption of transient product of, in radiolysis of nickel(II) porphyrin in various medium, 1-electron **oxidn.** process for)

RN 29484-62-6 CAPLUS
CN Nickel(1+), [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 133815-76-6 CAPLUS
CN Nickelate(3-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[benzenesulfonato]](6-)-N21,N22,N23,N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

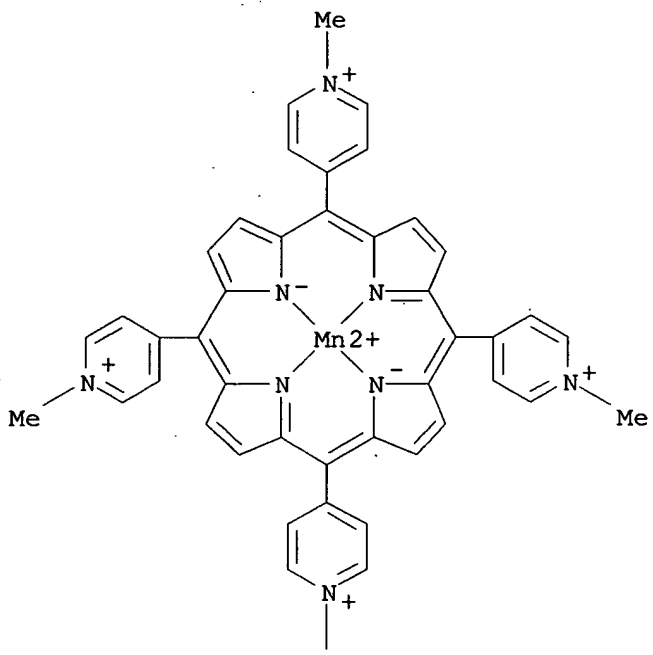


L6 ANSWER 23 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:428923 CAPLUS
DOCUMENT NUMBER: 109:28923
TITLE: Chemistry of a high-**oxidation**-level manganese porphyrin in aqueous solution
AUTHOR(S): Spreer, L. O.; Leone, Anthony; Maliyackel, A. C.; Otvos, J. W.; Calvin, Melvin
CORPORATE SOURCE: Lawrence Berkeley Lab., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Inorganic Chemistry (1988), 27(14), 2401-5
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mn(III) tetrakis(N-methyl-4-pyridiniumyl)porphyrin (MnIIIP+) (chloride salt) and other water-sol. manganese(III) porphyrins undergo facile one-electron electrochem. or chem. **oxidn**. in alk. soln. Best available evidence indicates that the final oxidized species is a Mn(IV) .mu.-oxo dimer, PMnIV-O-MnIVP2+. This same species is also produced by the reaction of manganese(II) porphyrin and oxygen. The Mn(IV) .mu.-oxo dimer has limited stability in water returning to 90-94% of the original Mn(III) porphyrin. The rate of this reaction is pH dependent with faster rates at lower pH. Oxygen is not produced during this redn. process. Rather, the reaction involves an unusual disproportionation in which a small percentage of the porphyrin macrocycles supply multiple electrons to reduce the remainder of the oxidized dimer. The Mn(IV) dimer reacts rapidly with water-sol. olefins as it also does in **aprotic** solvents. A mechanism for the disproportionation reaction is discussed with a rate-detg. step involving rearrangement of charge within the sym. dimer to one with both **oxidn**. equiv. on one metalloporphyrin unit, viz., PMnIV-O-MnIIIP+ or PMnIII-O-MnIIIP2+. This species undergoes nucleophilic attack by water or hydroxide, producing an isoporphyrin or bilirubin type mol. that has many olefinic bonds capable of reaction with remaining Mn(IV) .mu.-oxo dimer. Since coordination by OH- to the Mn center favors the higher Mn(IV) **oxidn**. level, the pH dependence of the disproportionation can be explained by rearrangement within the dimer to a porphyrin-centered **oxidn**. site.

IT **114595-73-2**
RL: PRP (Properties)
(chem. and electrochem. formation and disproportionation and reactions

PAGE 1-A



PAGE 2-A

L6 ANSWER 24 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:614190 CAPLUS
DOCUMENT NUMBER: 107:214190
TITLE: Chemistry of singlet oxygen. 48. Isolation and structure of the primary product of photooxygenation of 3,5-di-t-butyl catechol
AUTHOR(S): Jensen, Frank; Foote, Christopher S.
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. California, Los Angeles, CA, 90024, USA
SOURCE: Photochemistry and Photobiology (1987), 46(3), 325-30
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:214190

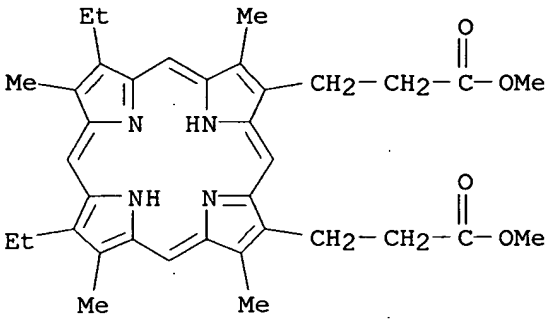
AB The dye-sensitized photooxygenation of t-butyl-substituted catechols has been investigated. The primary product from 3,5-di-t-butylcatechol has been isolated and shown to be a hydroperoxydienone by single crystal x-ray diffraction. The absence of sensitizer effects and the faster reaction rate in polar solvents suggest that the reaction proceeds with singlet O as the primary oxygenating species. Charge-transfer or full

electron-transfer from the catechol to singlet O is probably involved. Substituent effects are in agreement with this mechanism. The products from thermal breakdown of the hydroperoxydienone are inconsistent with a Baeyer-Villiger mechanism.

IT **1263-63-4**, Mesoporphyrin IX dimethyl ester
RL: BIOL (Biological study)
(photosensitization by, of butylcatechols photooxygenation)

RN 1263-63-4 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1987:543594 CAPLUS

DOCUMENT NUMBER: 107:143594

TITLE: Electrochemistry and properties of poly-p-phenylene formed from the anodic **oxidation** of biphenyl in **aprotic** solvents

AUTHOR(S): McAleer, Jerome F.; Ashley, Kevin; Smith, Jerry J.; Bandyopadhyay, Saibal; Ghoroghchian, Jamal; Eyring, Edward M.; Pons, Stanley; Mark, H. B., Jr.; Dunmore, Gordon

CORPORATE SOURCE: At. Energy Res. Establ., Harwell/Didcot/Oxfordshire, UK

SOURCE: Journal of Molecular Electronics (1986), 2(4), 183-91
CODEN: JMELE4; ISSN: 0748-7991

DOCUMENT TYPE: Journal

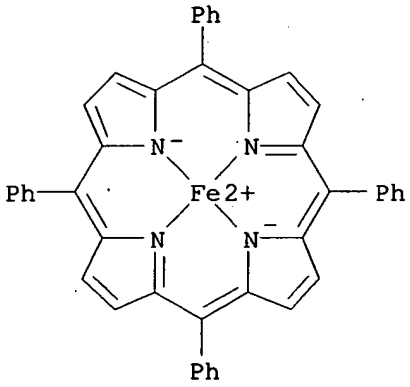
LANGUAGE: English

AB Conducting poly-p-phenylene films were grown on Pt electrodes via the electrochem. anodic polymn. of biphenyl. Electroreflectance and complex plane impedance anal. are used to investigate the cond. of the polymer which, like polypyrrole, is high for the oxidized and low for the neutral polymer. Films formed in this way have potential applications in batteries and are able to incorporate certain reactive species in a matrix that are useful for electrocatalysis.

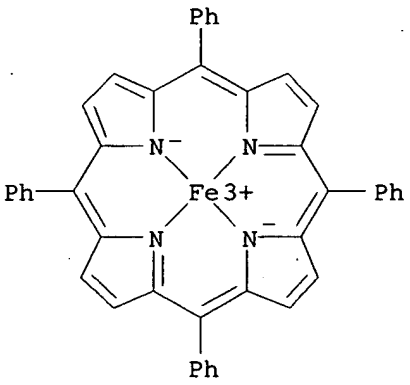
IT **16591-56-3**, Iron tetraphenylporphyrin **29484-63-7**
RL: PRP (Properties)
(cyclic voltammetry of trapped, in polyphenylene films)

RN 16591-56-3 CAPLUS

CN Iron, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 29484-63-7 CAPLUS
CN Iron(1+), [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



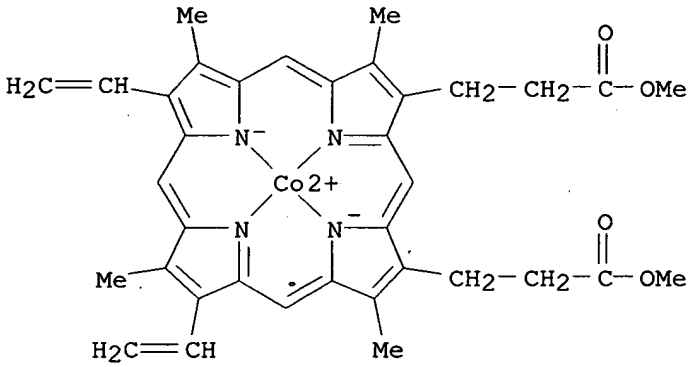
L6 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:202535 CAPLUS
DOCUMENT NUMBER: 106:202535
TITLE: Mechanism of reactions of cobalt(II) protoporphyrin IX dimethyl ester in protic and **aprotic**, co-ordinating solvents
AUTHOR(S): Pavlovic, Dusanka; Asperger, Smiljko; Domi, Bujar
CORPORATE SOURCE: Fac. Pharm. Biochem., Univ. Zagreb, Zagreb, Yugoslavia
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1986), (12), 2535-8
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Co(II) protoporphyrin IX di-Me ester (CoIIP), when dissolved in a coordinating, **aprotic**, highly dielec. solvent (S) in air, rapidly gives CoIIP(S) and CoIIP(S)(O2) at equil. The Soret absorption max. of these solns. gradually shift bathochromically, due probable to the formation of (S)CoIIIP(O2)CoIIIP(S) peroxo dimers. The Soret shifts and the reaction rate consts. as 25.degree. were detd. for DMSO, DMF,

hexamethylphosphoramide (HMPA), acetonitrile, and pyridine (py). The addn. of py to a soln. of CoIIP in MeOH accelerates the formation of CoIIIP(py)2+ until kobs. reaches 1.5 .times. 10-3 s-1. The disappearance of CoIIP then slows to a const. rate. Analogous rate max. appear with EtOH, CrOH, ethylene glycol and formamide. Addn. of py to the solns. of CoIIP DMSO or HMPA causes continuous increase of the rate of disappearance of CoIIP, indicating no formation of a bis(ligand) CoIIIP species.

IT **14932-10-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative and oxidative addn. reactions of, with pyridine and solvents, kinetics and mechanisms of)

RN 14932-10-6 CAPLUS

CN Cobalt, [dimethyl 7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



L6 ANSWER 27 OF 45 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1986:533609 CAPLUS

DOCUMENT NUMBER: 105:133609

TITLE: **Oxidation** of polyvalent porphyrin tetrakis(3,5-di-tert-butyl-4-hydroxyphenyl)porphyrin by superoxide ion

AUTHOR(S): Ozawa, Toshihiko; Hanaki, Akira

CORPORATE SOURCE: Natl. Inst. Radiol. Sci., Chiba, 260, Japan

SOURCE: Inorganica Chimica Acta (1985), 108(2), L11-L13
CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal

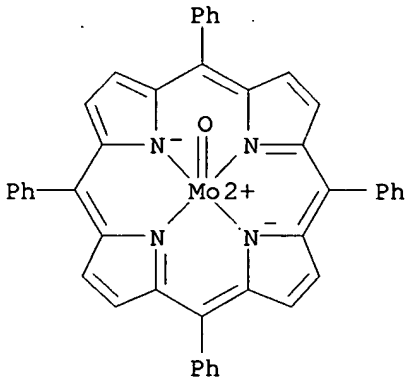
LANGUAGE: English

GI

TITLE: Reactions of molybdenum(V) tetraphenylporphyrins with superoxide. Mechanism of the reactions and the characterization of an isolated dioxygen complex
AUTHOR(S): Hasegawa, Koichi; Imamura, Taira; Fujimoto, Masatoshi
CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Inorganic Chemistry (1986), 25(13), 2154-60
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

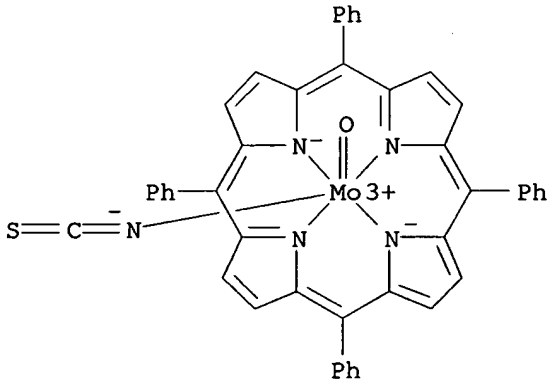
AB The mechanism of the reactions of MoVO(TPP)X (H2TPP = 5,10,15,20-tetraphenylporphyrin; X = Br, Cl, NCS) with O2- in **aprotic** solvents under anaerobic conditions was stoichiometrically elucidated. MoVO(TPP)X is reduced by O2- to MoIVO(TPP) in CH2Cl2 contg. 1% (vol./vol.) DMSO at 25.degree. via an intermediate complex. This intermediate is stable in soln. at -80.degree. but is converted into MoIVO(TPP) at room temp. and is ascertained to be [18-crown-6-K][MoVO(TPP)(O22-)] where the dioxygen binds side-on with the electronic configuration of peroxide. The structure and **oxidn.** state of the Mo-dioxygen unit in the dioxygen complex are maintained in **aprotic** media at -80 to -20.degree..

IT **33519-60-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from molybdenum pentavalent oxo complex with tetraphenylporphyrin and superoxide)
RN 33519-60-7 CAPLUS
CN Molybdenum, oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



IT **94782-05-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectrum of)
RN 94782-05-5 CAPLUS
CN Molybdenum(1+), oxo[sulfinylbis[methane]-O][5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-23)- (9CI) (CA INDEX NAME)

N21,N22,N23,N24](thiocyanato-N)-, (OC-6-32)- (9CI) (CA INDEX NAME)



L6 ANSWER 29 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:470893 CAPLUS
DOCUMENT NUMBER: 103:70893
TITLE: The **oxidation** of organic compounds with iodosylbenzene catalyzed by tetra(4-N-methylpyridyl)porphyrinatoiron(III) pentacation: a polar model system for the cytochrome P450 dependent monooxygenase
AUTHOR(S): Lindsay Smith, John R.; Mortimer, David N.
CORPORATE SOURCE: Dep. Chem., Univ. York, York, YO1 5DD, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1985), (7), 410-11
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:70893

AB A study of the epoxidn. of aliph. alkenes with PhIO showed that replacing the tetraphenylporphyrinatoiron(III) chloride [Fe(III)TPPCl] catalyst, in the model system Fe(III)TPPCl-PhIO (J. T. Groves, et al., 1979) for cytochrome P 450 monooxygenases, with tetra(4-N-methylpyridyl)porphyrinatoiron(III) pentacation, allowed **oxidns.** to be performed in protic and dipolar **aprotic** solvents without significantly altering the reaction mechanisms.

IT **60489-13-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for iodosylbenzene **oxidn.** of aliph. alkenes)

RN 60489-13-6 CAPLUS
CN Iron(5+), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis[1-methylpyridiniumato]](2-)]-, (SP-4-1)- (9CI) (CA INDEX NAME)

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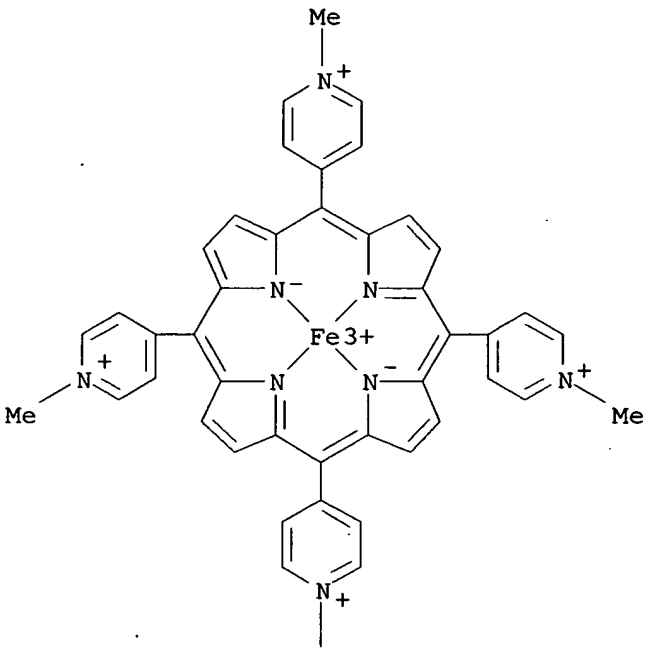

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L6 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:444684 CAPLUS
DOCUMENT NUMBER: 103:44684
TITLE: Electrochemical behavior of a binary cofacial dicobalt porphyrin in **aprotic** media under a nitrogen atmosphere. Formation of mixed-valence compounds
AUTHOR(S): Le Mest, Y.; L'Her, M.; Courtot-Coupez, J.; Collman, J. P.; Evitt, E. R.; Bencosme, C. S.
CORPORATE SOURCE: Fac. Sci. Tech., Univ. Bretagne Occident., Brest, 29283, Fr.
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1985), 184(2), 331-46
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English

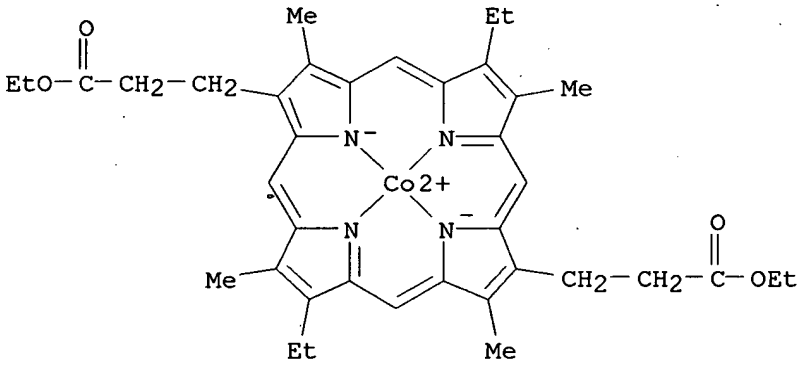
AB The electrochem. behavior of the binary cofacial dicobalt porphyrin (Co2FTF4) (FTF signifies face-to-face geometry of 2 Co atoms sepd. by 4-atom bridges) was investigated in benzonitrile under a pure N atm. The 2 Co(II) centers of the mol. are oxidized or reduced sep. in 2 different single-electron steps giving rise, for the 1st **oxidn**. and redn. reactions, to mixed-valence compds.: [CoIIICoII] and [CoIICoI], resp.; further **oxidn**. or redn. leads to the [CoIIICoIII] and [CoICoI]

derivs. All the redox systems are nearly reversible and diffusion-controlled, even the Co(III)/Co(II) ones. Except for the [CoICoI] species, all the redox states of the dicobalt bis porphyrin were generated by electrolysis and characterized by spectrophotometry and/or ESR spectroscopy. Whereas the [CoIICoII] compd. displays metal-metal interaction, the [CoIIICoII] is a valence-localized mixed-valence compd., i.e., the odd electron is localized on 1 Co. Such multistep charge transfers for the 2 nearly equiv. Co nuclei of the mol. are explained by the existence of interactions between the 2 Co(II) centers. The proximity of the 2 Co(II) atoms induces different properties of the Co2FTF4 porphyrin with regard to Co monoporphyrins.

IT **81849-14-1**
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(cyclic voltammetry of, at glassy carbon in benzonitrile, effect of methylimidazole on)

RN 81849-14-1 CAPLUS

CN Cobalt, [diethyl 7,17-diethyl-3,8,13,18-tetramethyl-21H,23H-porphine-2,12-dipropanoato(2-)-N21,N22,N23,N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

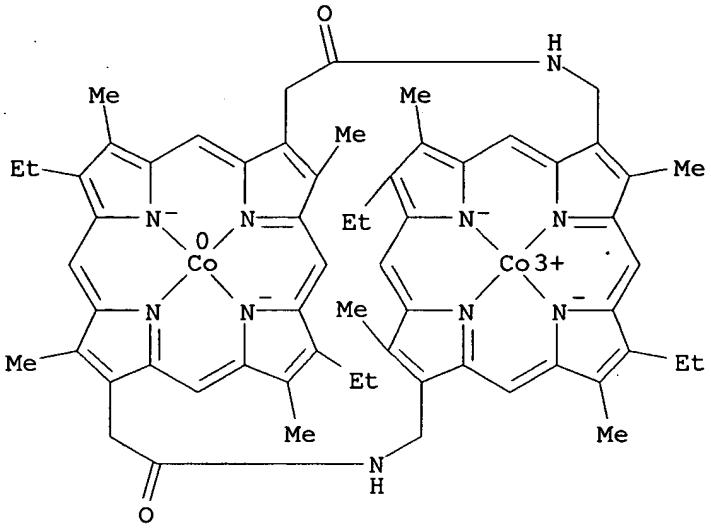


IT **96610-73-0**
RL: PRP (Properties)
(electrochem. formation and **oxidn.** on glassy carbon in benzonitrile and spectra of)

RN 96610-73-0 CAPLUS

CN Cobaltate(2-), [.mu.-[14,31,41,49-tetraethyl-4,5,23,24-tetrahydro-3,15,20,32,36,42,48,52-octamethyl-39H,46H-13,16:30,33-diimino-11,8:28,25-dimetheno-2,26:9,19-bis(metheno[2,5]-endo-pyrrolometheno)dipyrrolo[2,3-m:2',3'-c1][1,5,16,21]tetraazacyclodotriacontine-6,22(7H,21H)-dionato(4-)-N1,N27,N35,N39:N10,N18,N46,N51]]di- (9CI) (CA INDEX NAME)

3,15,20,32,36,42,48,52-octamethyl-39H,46H-13,16:30,33-diimino-11,8:28,25-dimetheno-2,26:9,19-bis(metheno[2,5]-endo-pyrrolometheno)dipyrrolo[2,3-m:2',3'-c1][1,5,16,21]tetraazacyclodotriacontine-6,22(7H,21H)-dionato(4-)-N1,N27,N35,N39:N10,N18,N46,N51]]di- (9CI) (CA INDEX NAME)



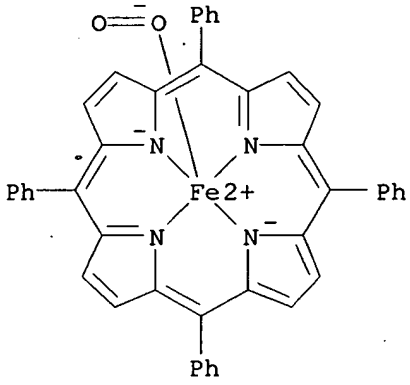
L6 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:625688 CAPLUS
DOCUMENT NUMBER: 101:225688
TITLE: The **oxidation** of hydrocarbons by peroxo complexes of metalloporphyrins in the presence of acylating agents. Modeling of the reaction of hydroxylation with the participation of cytochrome P-450
AUTHOR(S): Khenkin, A. M.; Shteinman, A. A.
CORPORATE SOURCE: Inst. Chem. Phys., Chernogolovka, 142432, USSR
SOURCE: Oxidation Communications (1983), 4(1-4), 433-41
CODEN: OXCODW; ISSN: 0209-4541
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The **oxidn**. of cyclohexane to cyclohexanol has been found to occur preferentially in **aprotic** solvents (C6H6, acetonitrile) at 20.degree. when the peroxo complexes of Fe(III)- or Mn(III)-tetraphenylporphyrin (TPP) are affected by acetic anhydride. The soln. of KO2 in C6H6 or acetonitrile also oxidizes cyclohexane under the action of acetic anhydride, but cyclohexanol and cyclohexanone are formed as **oxidn**. products in equal concns. To elucidate the reaction mechanism, the **oxidn**. of cis-trans-1,2-dimethylcyclohexane, isopentane, and cyclohexene has been studied in the systems [TPPFe(O2)]--Ac2O, KO2-Ac2O, and FeIIITPPCl-AcOOH. When hydroxylating dimethylcyclohexane in the presence of the peroxo complex, a partial retention of the original configuration (80%) is obsd., whereas with KO2 there is no retention of the conformation, which suggests a free radical mechanism of **oxidn**. in the system KO2-Ac2O. **Oxidn**. of cyclohexene in the system [TPPFe(O2)]--Ac2O results in formation of cyclohexenol-1 and cyclohexane oxide. In the system FeTPPCl-AcOOH,

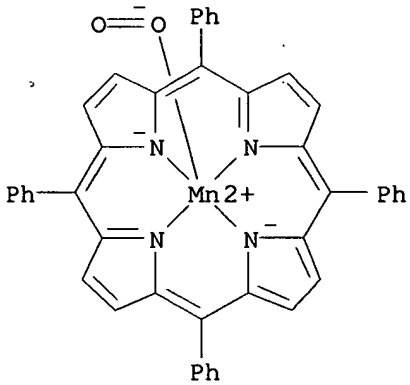
cyclohexane oxide is the only product, which indicates the different nature of the active intermediates in these 2 systems. The **oxidn**. of cyclohexane in the system [TPPFe(O2)]--acylating agent is independent of the nature of the anhydride (acetic anhydride, propionylchloride, ethylchloroformiate). The reaction of [TPPFe(O2)]- with Ac2O in toluene at -70.degree. has given an intermediate whose visible spectrum is consistent with the formula TPPFe-OOAc. A mechanism is proposed for the hydrocarbon **oxidn**. which includes acylation of the peroxo complex to the peracetate of Fe(III)-porphyrine, and decompn. of the complex to the oxoferrylporphyrine cation radical [(TPP)FeIV:O]+ which is responsible for the **oxidn**. of hydrocarbons. The newly discovered reaction and the hydroxylation mechanism of cytochrome P 450-contg. monooxygenases are compared.

IT **83160-26-3 83160-27-4 93365-70-9**
RL: BIOL (Biological study)
(in cytochrome P 450-contg. monooxygenase reaction model)

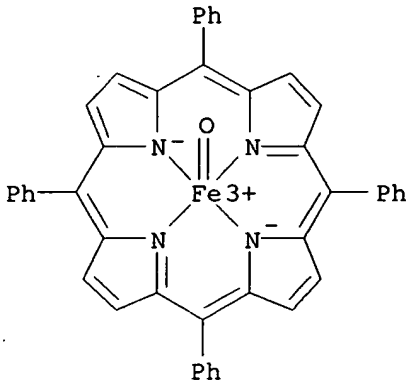
RN 83160-26-3 CAPLUS
CN Ferrate(1-), superoxido[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



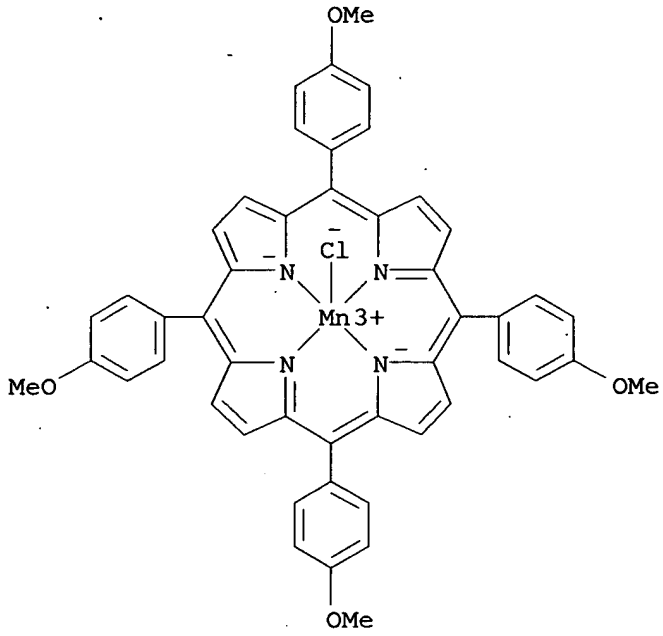
RN 83160-27-4 CAPLUS
CN Manganate(1-), superoxido[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



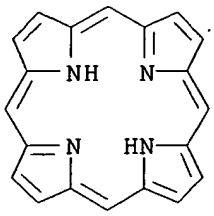
RN 93365-70-9 CAPLUS
CN Iron(1+), oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



L6 ANSWER 32 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:552174 CAPLUS
DOCUMENT NUMBER: 101:152174
TITLE: Effect of neutral salts on the kinetics of cholesterol **oxidation** in the presence of tetra-p-methoxyphenylporphyrinmanganese chloride-sodium borohydride
AUTHOR(S): Solov'eva, A. B.; Lukashova, E. A.; Karakozova, E. I.; Karmilova, L. V.; Nikiforov, G. A.; Enikolopyan, N. S.
CORPORATE SOURCE: Inst. Khim. Fiz., Moscow, USSR
SOURCE: Doklady Akademii Nauk SSSR (1984), 274(4), 858-61 [Phys. Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Kinetics were detd. for the oxygen **oxidn.** of cholesterol to give 5.alpha.-cholestane-3.beta.,5-diol in the presence of tetrakis(4-methoxyphenyl)porphyrin-MnCl-NaBH4 catalyst and with added salts, i.e. LiCl, LiBr, LiF, LiClO4, KCl, and CaCl2. The rate of **oxidn.** decreased linearly with increasing salt concn., and this rate redn. was less in the **aprotic** solvent Diglyme than in EtOH. A proposed reaction mechanism involved complexation of added salt with the catalyst.
IT **62769-24-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalyst contg. sodium borohydride and, for **oxidn.** of cholesterol)
RN 62769-24-8 CAPLUS
CN Manganese, chloro[5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



L6 ANSWER 33 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:434801 CAPLUS
DOCUMENT NUMBER: 101:34801
TITLE: The electrochemistry of strapped and capped porphyrin monomers, mono- and doubly-linked dimers, and their zinc and magnesium complexes
AUTHOR(S): Becker, J. Y.; Dolphin, D.; Paine, J. B.; Wijesekera, T.
CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1984), 164(2), 335-46
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effects of distortion, steric hindrance, distance, and orientation exerted by a variety of porphyrin monomers (strapped and capped) and dimers (singly- and doubly-linked) on the porphyrin redox properties as well as the stability of pos. charged intermediates derived from them were studied. Cyclic voltammograms were obtained in **aprotic** media for both the free bases and their metal complexes (Zn and Mg). The effect of the nature of supporting electrolyte on the anodic peak potentials and wave sepn. was studied in the case of conjugated directly-linked bis(Zn) and bis(Mg) porphyrins.
IT **87280-58-8 87280-60-2 87280-61-3**
90894-73-8 90894-74-9 90894-75-0
90894-76-1 90894-77-2 90894-78-3
90894-79-4 90894-80-7 90894-81-8
90894-82-9 90894-83-0 90894-84-1
90894-85-2 90894-86-3 90894-87-4
90894-88-5 90894-89-6 90894-90-9
90894-91-0 90895-04-8 90901-30-7

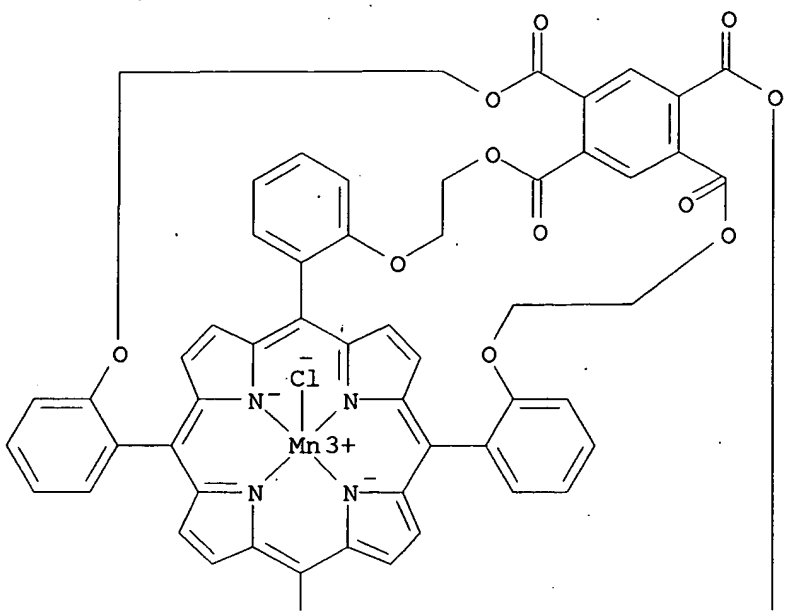


L6 ANSWER 34 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:205616 CAPLUS
DOCUMENT NUMBER: 100:205616
TITLE: Study of (tetraphenylporphinato)manganese(III)-catalyzed epoxidation and demethylation using p-cyano-N,N-dimethylaniline N-oxide as oxygen donor in a homogeneous system. Kinetics, radiochemical ligation studies, and reaction mechanism for a model of cytochrome P-450
AUTHOR(S): Powell, Michael F.; Pai, Emil F.; Bruice, Thomas C.
CORPORATE SOURCE: Dep. Chem., Univ. California, Santa Barbara, CA, 93106, USA
SOURCE: Journal of the American Chemical Society (1984), 106(11), 3277-85
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

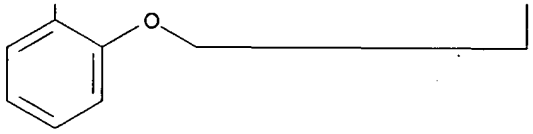
AB O transfer from p-cyanodimethylaniline N-oxide (I) to cyclohexene as well as intramol. O transfer accompanied by demethylation to yield p-cyanomonomethylaniline (II) are strongly catalyzed by ligated (tetraphenylporphinato)MnIII (i.e., XMnIIITPP). These reactions were studied in dry, O2-free benzonitrile. Radiochem. studies show that H2O (or TOH) is not bound to XMnIIITPP in **aprotic** solvents so that the MnIII moiety is pentacoordinate. O transfer occurs through the reversible formation of the hexacoordinated species I.cntdot.MnIII(X)TPP. This species decomps. to p-cyanodimethylaniline and O=MnV(X)TPP. The reaction of cyclohexene with O=MnV(X)TPP yields cyclohexene epoxide and XMnIIITPP, whereas II is formed directly from the I.cntdot.MnIII(X)TPP complex. The rates of product formation are shown to be dependent upon the nature of the ligand (X = F-, Cl-, Br-, I-, OCN-). In the absence of the axial ligand X, the rates of reaction are extremely slow. Thus, the MnIII C2-cap-porphyrin (XMnIIICAPTPP), which can only form an O=MnV porphyrin species wherein the Mn moiety is not complexed to X as a 6th ligand, shows almost no tendency to act as a catalyst for O transfer. The necessary presence of the axial ligand X and the dependence of rate and product upon X requires the structure of the O-transfer species to be equiv. to O=MnV(X)TPP. A kinetic anal. is presented which has allowed the detn. of the influence of the ligands X on the various rate consts. involved in the overall **oxidns**. By employing I as O donor, multiple catalytic turnovers without loss of porphyrin were realized.

IT **32195-55-4P 55290-32-9P 55290-33-0P**
56413-47-9P 86549-48-6P 89789-33-3P
89789-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction kinetics with cyanodimethylaniline N-oxide in presence of cyclohexene)

PAGE 1-A



PAGE 2-A

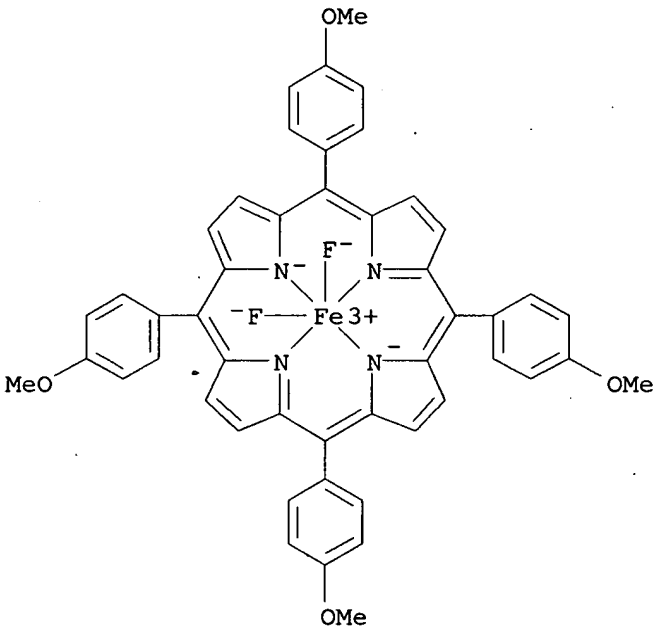


L6 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:532672 CAPLUS
DOCUMENT NUMBER: 99:132672
TITLE: Characterization of a unique electrochemical **oxidation** catalyst: the difluoro complex of iron(III) tetraphenylporphyrin
AUTHOR(S): Hickman, David L.; Goff, Harold M.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Inorganic Chemistry (1983), 22(20), 2787-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two F- ions bind with high affinity to Fe(III) porphyrins in **aprotic** solvents forming 6-coordinate anionic high-spin complexes. NMR, ESR, and soln. magnetic measurements clearly demonstrate the high-spin Fe(III) character of the difluoro complex. The 1H NMR spectrum of [Fe(TPP)F2]- (H2TPP = tetraphenylporphyrin) indicates a plane of symmetry in the porphyrin plane implying trans-F ligation. This complex has unique electrochem. properties in that the species is oxidized at 0.45

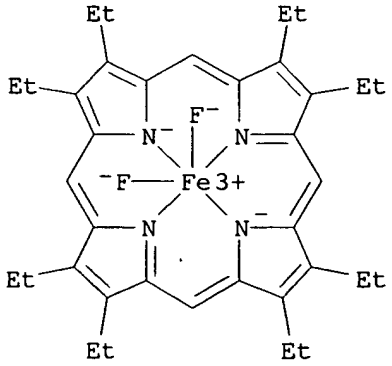
V less anodic than that of other 5-coordinate high-spin Fe(III) tetraphenylporphyrin complexes. The resulting oxidized difluoro-complex is short-lived in CH2Cl2 soln. This high reactivity was exploited by demonstrating that the difluoro-complex can serve as a catalyst for the electrochem. **oxidn**. of cyclohexene to the alc., ketone, and epoxide.

IT **86646-34-6 86668-09-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ESR triplet structure of)

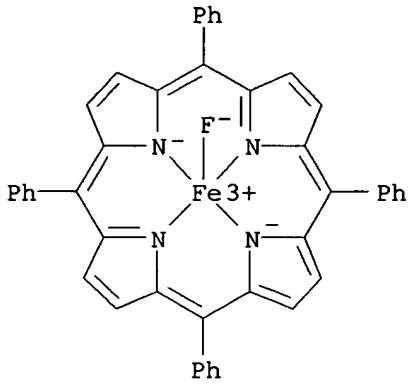
RN 86646-34-6 CAPLUS
CN Ferrate(1-), difluoro[5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)- (9CI) (CA INDEX NAME)



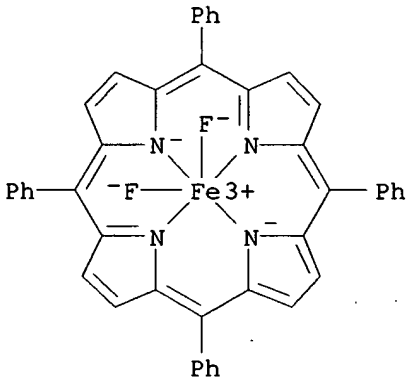
RN 86668-09-9 CAPLUS
CN Ferrate(1-), difluoro[2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)- (9CI) (CA INDEX NAME)



IT **55428-47-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(NMR and reaction and binding const. with tetrabutylammonium fluoride)
RN 55428-47-2 CAPLUS
CN Iron, fluoro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



IT **76402-68-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(characterization and use as electrochem. **oxidn**. catalyst)
RN 76402-68-1 CAPLUS
CN Ferrate(1-), difluoro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (OC-6-12)- (9CI) (CA INDEX NAME)



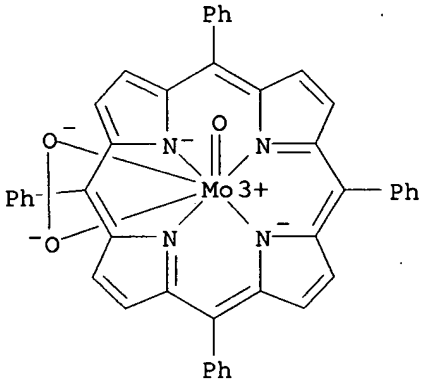
L6 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:415497 CAPLUS
DOCUMENT NUMBER: 99:15497
TITLE: Intermediate in the reaction of oxomolybdenum(V) tetraphenylporphyrin complex with superoxide ion in **aprotic** solvents
AUTHOR(S): Imamura, Taira; Hasegawa, Koichi; Fujimoto, Masatoshi
CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Chemistry Letters (1983), (5), 705-8
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English

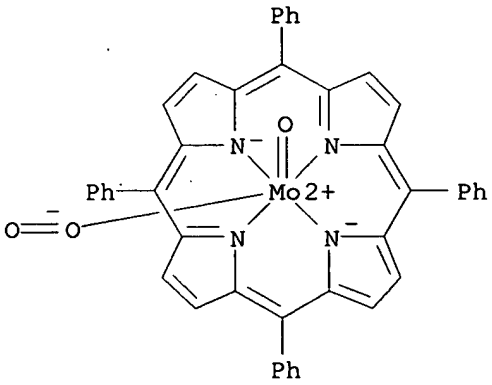
AB MoVO(tpp)Br (H2tpp = meso-tetraphenylporphine) is reduced by O2- to MoIVO(tpp) in 1% (vol./vol.) DMSO-CH2Cl2 medium at 25 .degree. via an intermediate. The intermediate is suggested on the basis of ESR and electronic spectral data to be a dioxygen complex and stably exists in the soln. at - 72.degree. as [MoIVO(tpp)(O2)]-. The **oxidn.** state of the central molybdenum in the intermediate complex reversibly changes with temp. between 4+ at -80.degree. and 5+ at 0.degree..

IT **86158-76-1P 86167-58-0P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, as intermediate in the **oxidn.** of bromooxo(tetraphenylporphinato)molybdenum by superoxide ion)

RN 86158-76-1 CAPLUS
CN Molybdate(1-), oxoperoxy[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]- (9CI) (CA INDEX NAME)



RN 86167-58-0 CAPLUS
CN Molybdate(1-), oxosuperoxido[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-23)- (9CI) (CA INDEX NAME)

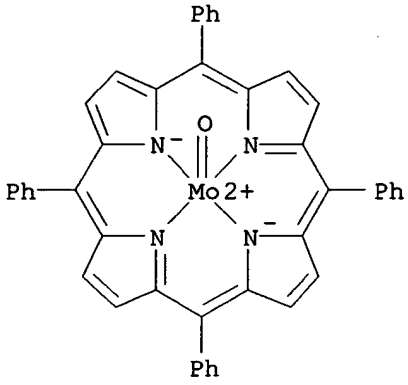


IT **33519-60-7P**

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from superoxide ion and bromooxo(tetraphenylporphinato)molybdenum)

RN 33519-60-7 CAPLUS

CN Molybdenum, oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)

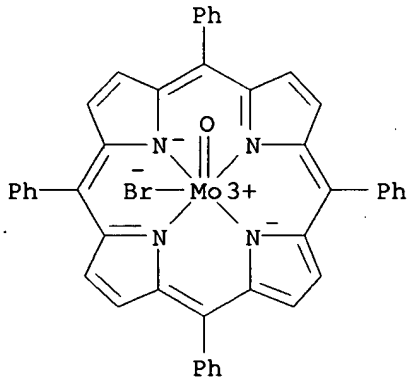


IT **73515-72-7**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with superoxide ion)

RN 73515-72-7 CAPLUS

CN Molybdenum, bromooxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (OC-6-23)- (9CI) (CA INDEX NAME)

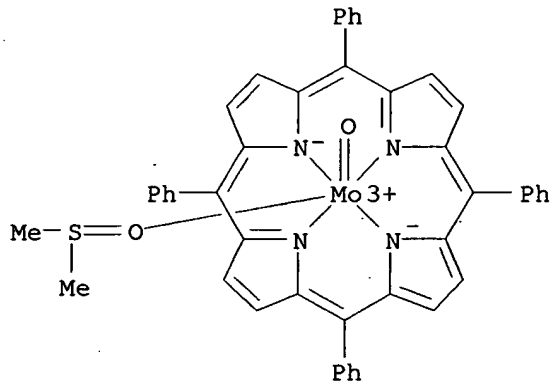


IT **86158-75-0**

RL: RCT (Reactant); RACT (Reactant or reagent)
(redox reaction with superoxide ion)

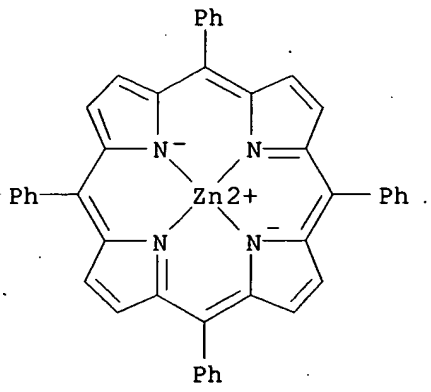
RN 86158-75-0 CAPLUS

CN Molybdenum(1+), oxo[sulfinylbis[methane]-O][5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, bromide, (OC-6-23)- (9CI) (CA INDEX NAME)



● Br^-

L6 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:44027 CAPLUS
DOCUMENT NUMBER: 98:44027
TITLE: Chemistry of singlet oxygen. 38. Temperature effect on the photooxidation of sulfides
AUTHOR(S): Gu, Chee Liang; Foote, C. S.
CORPORATE SOURCE: Dep. Chem., Univ. California, Los Angeles, CA, 90024, USA
SOURCE: Journal of the American Chemical Society (1982), 104(22), 6060-3
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reactivity of di-Et sulfide with singlet O was detd. at room temp. (23-24.degree.) and at -78.degree. in various solvents. Although the consumption of sulfide was much faster at -78.degree., the rate of removal of singlet O by sulfide was relatively independent of solvent and temp. A comparison of the rate of product formation with the rate of singlet O removal shows that over 97% quenching was obsd. in **aprotic** solvents and about 10% in protic solvents at room temp. At -78.degree., the quenching process was suppressed in both protic and **aprotic** solvents. 2,5-Diphenylfuran showed a similar but much smaller effect of solvent and temp.
IT **14074-80-7**
RL: USES (Uses)
(photolysis of system contg. oxygen and di-Et sulfide and, as sensitizer)
RN 14074-80-7 CAPLUS
CN Zinc, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

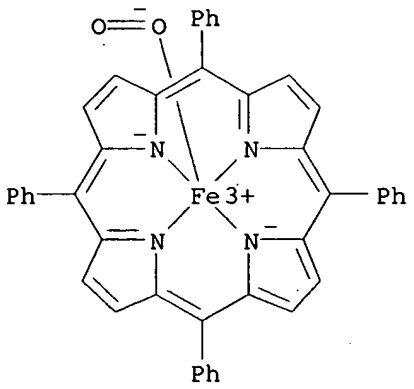


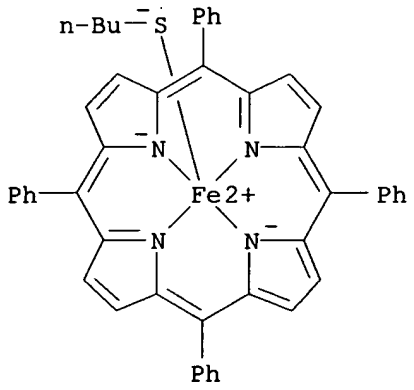
L6 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1982:416046 CAPLUS
DOCUMENT NUMBER: 97:16046
TITLE: Structure and chemical properties of products of the reaction of hemes with oxygen O-2.cntdot.
AUTHOR(S): Khenkin, A. M.; Shteinman, A. A.
CORPORATE SOURCE: Inst. Khim. Fiz., Chernogolovka, USSR
SOURCE: Kinetika i Kataliz (1982), 23(1), 219-22
CODEN: KNKTA4; ISSN: 0453-8811
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB ESR, Moessbauer spectral, magnetic susceptibility data, chem. behavior, and thermodn. relations confirm that the products of the reaction of hemes with O2.cntdot.- are peroxy complexes of high-spin Fe(III)-porphyrins. In **aprotic** solvents and in the presence of acid these compds. do not have oxidizing capabilities with respect to hydrocarbons but can oxidize cyclohexane with treatment with Ac2O.

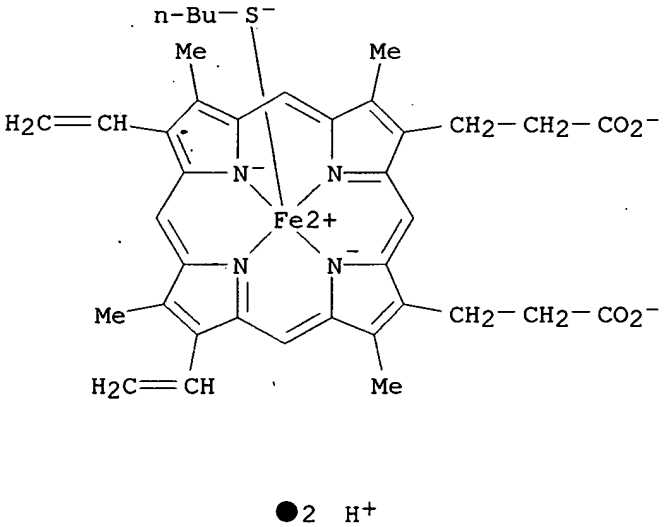
IT **67887-55-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ESR of)

RN 67887-55-2 CAPLUS
CN Iron, superoxido[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)





RN 77773-03-6 CAPLUS
CN Ferrate(3-), (1-butanethiolato)[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-N21,N22,N23,N24]-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)

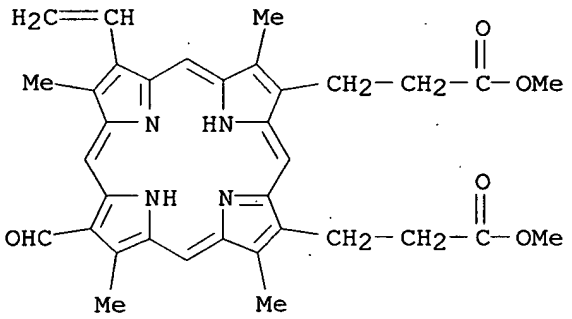


L6 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1982:43740 CAPLUS
DOCUMENT NUMBER: 96:43740
TITLE: Mechanisms for the photooxidation of protoporphyrin IX in solution
AUTHOR(S): Cox, G. Sidney; Whitten, David G.
CORPORATE SOURCE: Dep. Chem., Univ. North Carolina, Chapel Hill, NC, 27514, USA
SOURCE: Journal of the American Chemical Society (1982), 104(2), 516-21
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

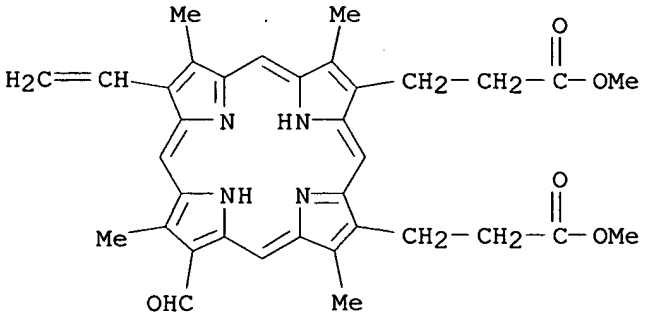
AB Protoporphyrin IX di-Me ester (I) is photooxidized upon irradn. in **aprotic** org. solvents in the presence of O to yield a mixt. of hydroxy aldehydes (photoprotoporphyrins), monoformylmonovinyldeuteroporphyrins, and diformyldeuteroporphyrin. Studies of the reactions under a variety of conditions show that major proportion of all of these products arises via a singlet O path. The formyl products can also arise via reaction of the protoporphyrin .pi. cations with superoxide, but this path can be shown to be of only minor importance when only the porphyrin and O are involved in direct irradn. of the porphyrin. Quenching of singlet O by ground-state I occurs with a rate const. kp = 8.5 .times. 105 M-1 s-1; this value is comparable to that measured for other free-base porphyrins but considerably lower than that obsd. for open-shell metalloporphyrins and for free-base chlorins. The relatively low limiting quantum yield obtained for reaction of I indicates that net phys. quenching is the result of most porphyrin-singlet O interactions.

IT **10200-04-1P 13187-15-0P 15341-25-0P**
RL: PREP (Preparation)
(formation and yield of, in photooxidn. of protoporphyrin IX in soln.)

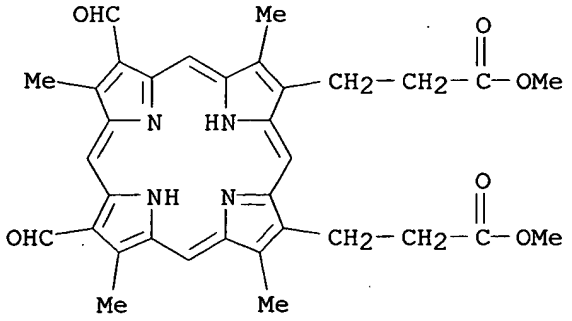
RN 10200-04-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7-ethenyl-12-formyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



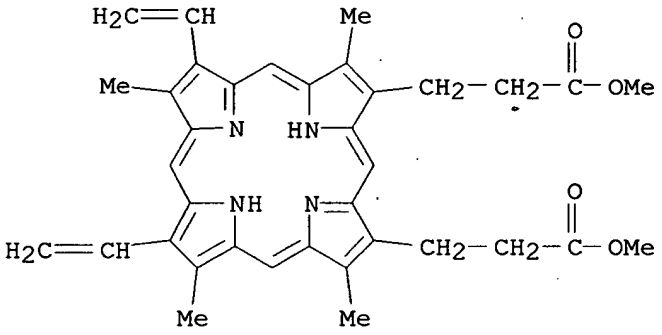
RN 13187-15-0 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 8-ethenyl-13-formyl-3,7,12,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 15341-25-0 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diformyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



IT **5522-66-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photooxidn. of, in org. soln., mechanism of)
RN 5522-66-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

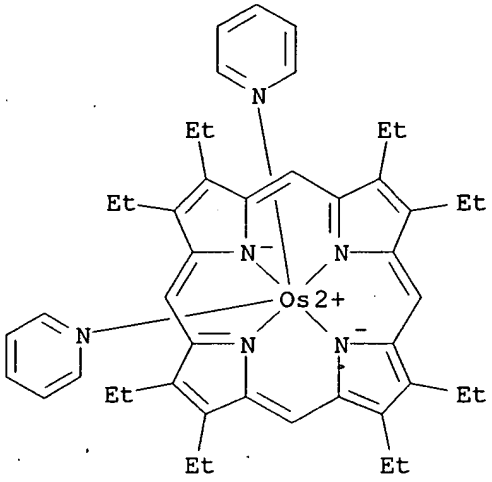


L6 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:169880 CAPLUS
DOCUMENT NUMBER: 94:169880
TITLE: Production of superoxide by osmochromes
AUTHOR(S): Buchler, J. W.; Billecke, J.; Kokisch, W.
CORPORATE SOURCE: Fachber. Anorg. Chem. Kernchem., Tech. Hochsch. Darmstadt, Darmstadt, D-6100, Fed. Rep. Ger.
SOURCE: Developments in Biochemistry (1980), 11A(Chem. Biochem. Aspects Superoxide Superoxide Dismutase), 45-55
CODEN: DEBIDR; ISSN: 0165-1714
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A substitutionally inert osmochrome, bis(1-methylimidazole)-octaethylporphinatoosmium(II), produces appreciable amts. of O2- by direct outer-sphere electron transfer to O2 in pyridine-water (99:1) as evidenced by EPR. The subsequent dismutation of O2- to O2 and H2O2 (detected as the peroxotitanyl complex) constitutes the acid-induced autoxidn. of osmochromes which are air-stable in **aprotic** solvents because

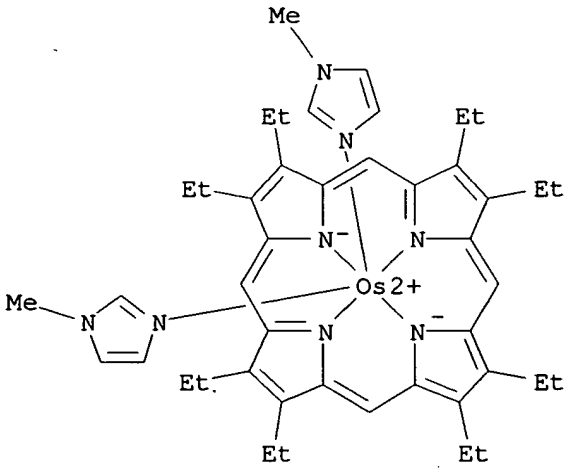
they do not offer a coordination site for the O2 mol. This reaction sequence is suggested for the autoxidn. of hemochromes in pyridine/acid or H2O, or of cytochromes b. The stoichiometry of the autoxidn. is followed by respirometry. In the absence of H2O, O2- reduces osmichrome salts to osmochromes.

IT **51286-87-4 74077-51-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(autoxidn. of, superoxide formation in relation to)

RN 51286-87-4 CAPLUS
CN Osmium, [2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]bis(pyridine)-, (OC-6-12)-(9CI) (CA INDEX NAME)



RN 74077-51-3 CAPLUS
CN Osmium, bis(1-methyl-1H-imidazole-N3)[2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)- (9CI) (CA INDEX NAME)

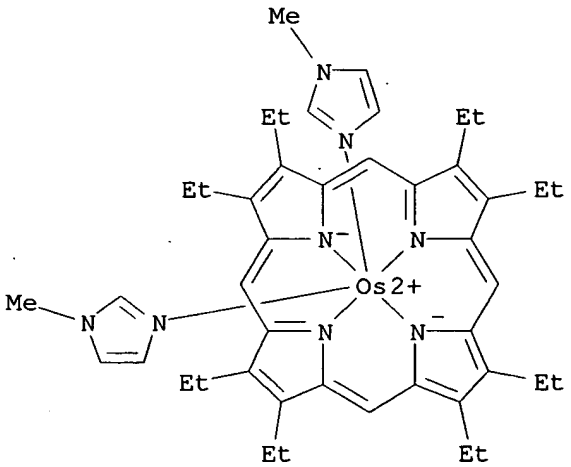


L6 ANSWER 41 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1980:421049 CAPLUS
DOCUMENT NUMBER: 93:21049
TITLE: Osmochromes (osmium analogs of hemochromes): proof of superoxide and hydroperoxide generation from dioxygen and a metalloporphyrin lacking a free coordination site
AUTHOR(S): Billecke, Jochen; Kokisch, Wolfgang; Buchler, J. W.
CORPORATE SOURCE: Inst. Anorg. Chem., Tech. Hochsch. Aachen, Aachen, D-5100, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1980), 102(10), 3622-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A substitutionally inert osmochrome, bis(1-methylimidazole)octaethylporphinatoosmium(II), produced appreciable amts. of O2- by direct outer-sphere electron transfer to O2 in pyridine-water (99:1) as evidenced by EPR. The subsequent dismutation of O2- to O2 and H2O2 (detected as the peroxotitanyl complex) constituted the acid-induced autoxidn. of osmochromes which were air-stable in **aprotic** solvents because they did not offer a coordination site for the O2 mol. This reaction sequence is suggested for the autoxidn. of hemochromes in pyridine/acid or water, or of cytochromes b. The stoichiometry of the autoxidn. was followed by respirometry. In the absence of water, O2- reduced osmichrome salts to osmochromes.

IT **74077-51-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(autoxidn. of, mechanism of, cytochromes and hemochromes in relation to)

RN 74077-51-3 CAPLUS
CN Osmium, bis(1-methyl-1H-imidazole-N3)[2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (OC-6-12)- (9CI) (CA INDEX NAME)



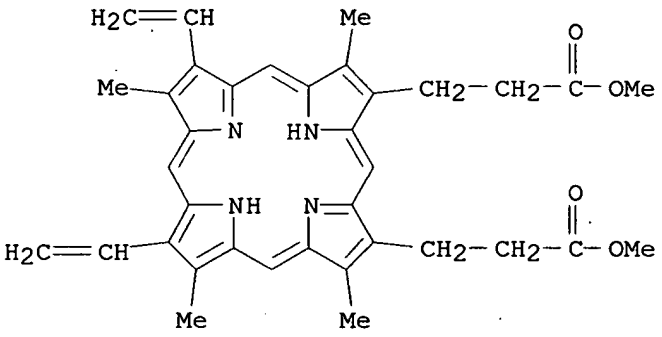
L6 ANSWER 42 OF 45 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1980:180355 CAPLUS
DOCUMENT NUMBER: 92:180355
TITLE: Interaction of porphyrin and metalloporphyrin excited states with molecular oxygen. Energy-transfer versus electron-transfer quenching mechanisms in photo **oxidations**
AUTHOR(S): Cox, G. Sidney; Whitten, David G.; Giannotti, Charles
CORPORATE SOURCE: Dep. Chem., Univ. North Carolina, Chapel Hill, NC, 27514, USA
SOURCE: Chemical Physics Letters (1979), 67(2-3), 511-15
CODEN: CHPLBC; ISSN: 0009-2614
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The quenching of porphyrin and metalloporphyrin excited states by O2 in protic and **aprotic** org. solvents is reported. Studies using spin traps in the ESR together with an investigation of photooxidn. behavior indicate that both superoxide ion and singlet O2 are formed in the quenching process for several porphyrins. For Pd octaethylporphyrin irreversible branching occurs in the quenching prior to the formation of free superoxide.

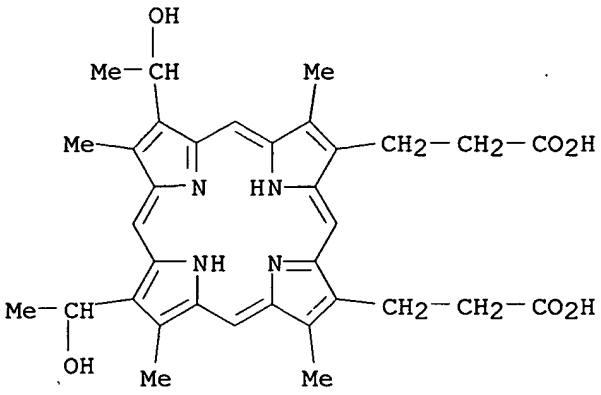
IT **5522-66-7 14074-80-7 14187-13-4 14187-14-5 14459-29-1 24804-00-0**
RL: PRP (Properties)
(quenching of excited state of, mechanism of)

RN 5522-66-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)

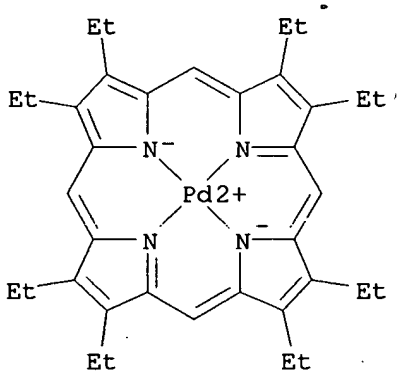


RN 14074-80-7 CAPLUS
CN Zinc, [5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)

RN 14459-29-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 24804-00-0 CAPLUS
CN Palladium, [2,3,7,8,12,13,17,18-octaethyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



L6 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1978:580568 CAPLUS
DOCUMENT NUMBER: 89:180568
TITLE: Oxygenation of polymer-covalently bonded metalloporphyrins
AUTHOR(S): Tsuchida, Eishun; Hasegawa, Etsuo; Kanayama, Tatsuya
CORPORATE SOURCE: Dep. Polym. Chem., Waseda Univ., Tokyo, Japan
SOURCE: Macromolecules (1978), 11(5), 947-55
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of mol. O with Co(II) and Fe(II) complexes of styrene copolymers with protoporphyrin IX styrylamide [**67552-99-2**], 5-(4-acrylamidophenyl)-10,15,20-triphenylporphine [**67553-01-9**],

or 5,10,15,20-tetrakis(2-methacrylamidophenyl)porphine (I) [**67583-89-5**] in dry, **aprotic** solvents was studied by ESR and electronic spectra. O binding by the Co complexes was increased by bonding to the polymer, owing to desolvation of the porphyrins by steric restrictions. The polymer chain also prevented the complexes from dimerization and dimeric **oxidn.** at styrene-porphyrin mol ratio >1000. A slow, monomol. **oxidn.** occurred at room temp., which was most effectively inhibited by the amide groups of I, giving the most stable O adduct.

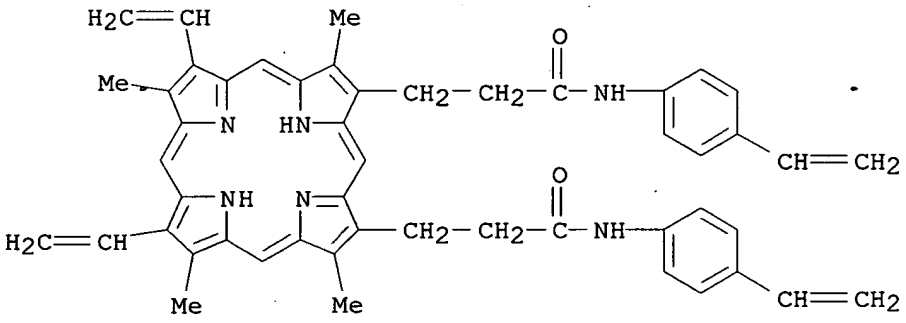
IT **66253-53-0D**, cobalt and iron complexes **67553-02-0D**, cobalt and iron complexes **67583-90-8D**, cobalt and iron complexes
RL: USES (Uses)
(mol. oxygen bonding by)

RN 66253-53-0 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanamide, 7,12-diethenyl-N,N'-bis(4-ethenylphenyl)-3,8,13,17-tetramethyl-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

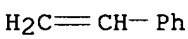
CM 1

CRN 66253-52-9
CMF C50 H48 N6 O2



CM 2

CRN 100-42-5
CMF C8 H8

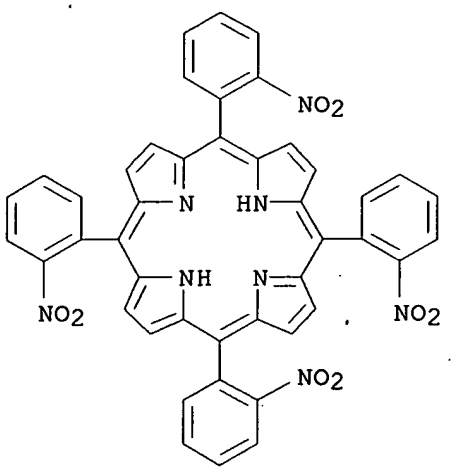


RN 67553-02-0 CAPLUS

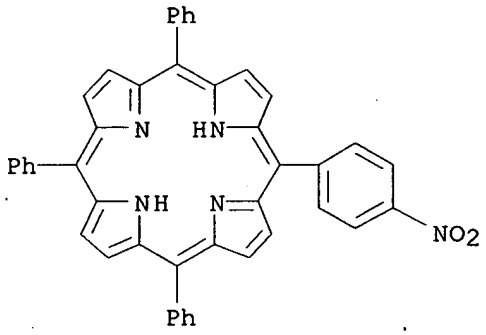
CN 2-Propenamide, N-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]-, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 67553-01-9
CMF C47 H33 N5 O



RN 67605-65-6 CAPLUS
CN 21H,23H-Porphine, 5-(4-nitrophenyl)-10,15,20-triphenyl- (9CI) (CA INDEX NAME)

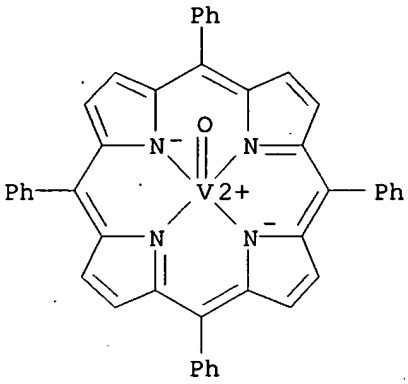


L6 ANSWER 44 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1976:81669 CAPLUS
DOCUMENT NUMBER: 84:81669
TITLE: ESR and electrochemical studies of some transition metal porphyrins
AUTHOR(S): Newton, Carolyn M.; Davis, Donald G.
CORPORATE SOURCE: Dep. Chem., Univ. New Orleans, New Orleans, LA, USA
SOURCE: Journal of Magnetic Resonance (1969-1992) (1975), 20(3), 446-57
CODEN: JOMRA4; ISSN: 0022-2364
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The techniques of cyclic voltammetry, controlled-potential coulometry and ESR were used to examine the mechanisms of the redox chem. of V(IV), Cr(III), Mo(V) and W(V) tetraphenylporphyrins (TPP). Various nonaq. **aprotic** solvents were used, esp. N,N-dimethylacetamide (DMA) and dichloromethane. One-electron metal redns. were obsd. for all of the complexes except V, as well as one-electron **oxidn**. of Cr(IV). Formation of .pi. anions and .pi. cations was detected resulting from the

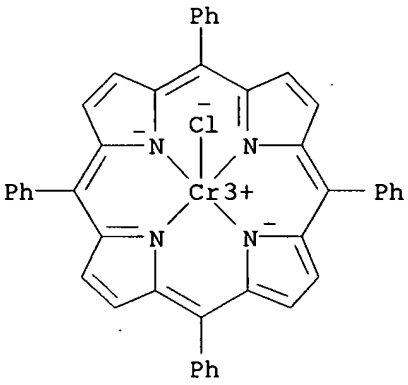
oxidn. or redn. of the porphyrin ring. The heterogeneous rate consts. for the various electrochem. reactions were detd. ESR studies revealed extrahyperfine interaction for the Cr and Mo complexes. The .pi. anion radical of V exhibited a relaxation mechanism by which the metal signal was broadened but the .pi. radical signal was not.

IT **14705-63-6 28110-70-5 28780-74-7 58441-02-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(redox reactions of, ESR and electrochem. techniques in relation to)

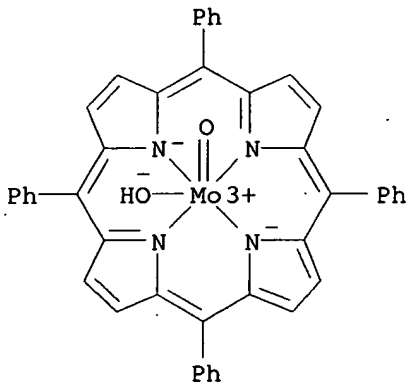
RN 14705-63-6 CAPLUS
CN Vanadium, oxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



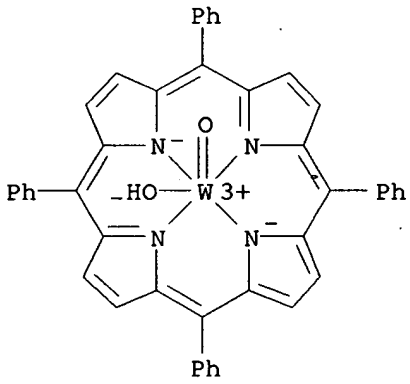
RN 28110-70-5 CAPLUS
CN Chromium, chloro[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)- (9CI) (CA INDEX NAME)



RN 28780-74-7 CAPLUS
CN Molybdenum, hydroxyoxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (OC-6-23)- (9CI) (CA INDEX NAME)



RN 58441-02-4 CAPLUS
CN Tungsten, hydroxyoxo[5,10,15,20-tetraphenyl-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (OC-6-23)- (9CI) (CA INDEX NAME)



L6 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1974:541489 CAPLUS
DOCUMENT NUMBER: 81:141489
TITLE: Solvent effects on reversible formation and oxidative stability of heme-oxygen complexes
AUTHOR(S): Brinigar, W. S.; Chang, C. K.; Geibel, J.; Traylor, T. G.
CORPORATE SOURCE: Dep. Chem., Univ. California, La Jolla, CA, USA
SOURCE: Journal of the American Chemical Society (1974), 96(17), 5597-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Heme compds. with either covalently linked bases, e.g., pyrroheme-[3-(1-.Imidazolyl)propyl]amide or pyrroheme-[3-(3-pyridyl)propyl]ester (I), or protoheme with excess 1-n-butylimidazole bind O in polar **aprotic** solvents. The oxygenation equil. const. in I increases about 100-fold when the solvent is changed from toluene to DMF. Stability toward **oxidn**. is also enhanced by this change. These results are interpreted in terms of a polar Fe-O2 bond.

L7 27 L4 AND DIAZEPAM?

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L7 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:928122 CAPLUS
DOCUMENT NUMBER: 138:12504
TITLE: Method for assaying biomolecules and other constituents using indicator conjugates with synthetic nucleounits in lateral flow, liquid, and dry chemistry techniques
INVENTOR(S): Smith, Jack V.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 46 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

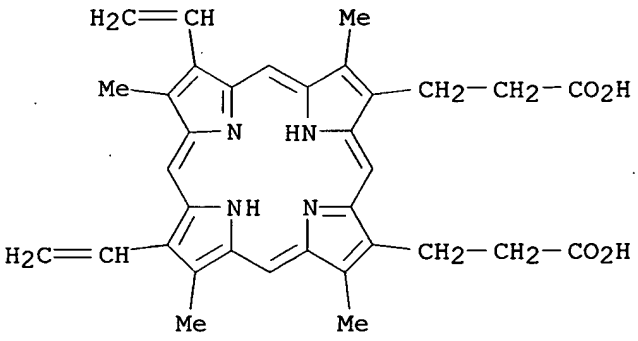
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002182600	A1	20021205	US 2001-829563	20010411

PRIORITY APPLN. INFO.: US 2001-829563 20010411

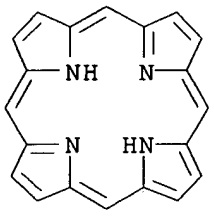
AB The present invention is a method for the use of particles made up of nucleotides or fragments of base groups of DNA and RNA mols. herein referred to as synthetic nucleounits which can be used as recognition mols. with specificity and sensitivity significantly greater than that of antibodies which are used in clin. diagnostics, biotechnol., and research. The method for detecting an analyte using nucleounits targeted to the analyte comprises (1) identifying a nucleounit from a mixt. of synthetic random sequences of nucleounit libraries, (2) conjugating the nucleounit to an indicator for the analyte, and (3) detecting the analyte using the nucleounit-indicator conjugate in a buffer. Step 1 is carried out by (a) contacting the analyte with the mixt. of synthetic random sequences of nucleounit libraries such that some nucleounits bind the analyte, (b) removing the unbound nucleounits by partitioning, and (c) amplifying the remaining nucleounits by PCR to obtain an enriched soln. of nucleounits with high affinity for the analyte. Thus, a method and lateral flow test strip for detection of cytomegalovirus (CMV) presence in a biol. sample such as serum or urine is described. The strip is prepd. with three solns., one contg. anti-CMV antibodies, one contg. "nucleounit to CMV antibody conjugated to red microparticles" and "red microparticles", and another contg. "nucleounit to colored particles". The "nucleounit" may be an oligonucleotide aptamer specific for anti-CMV antibodies.

IT **553-12-8**, Protoporphyrin **26316-36-9**, Uroporphyrin
27121-71-7, Coproporphyrin
RL: ANT (Analyte); ANST (Analytical study)
(method for assaying biomols. and other constituents using indicator conjugates with synthetic nucleounits in lateral flow, liq., and dry chem. techniques)

RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



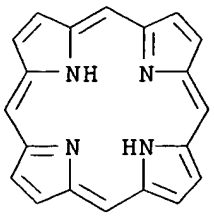
RN 26316-36-9 CAPLUS
CN 21H,23H-Porphine-C,C,C,2-tetrapropanoic acid, C,C,C,3-tetrakis(carboxymethyl)- (9CI) (CA INDEX NAME)



4 [D1—CH_2—CO_2H]

4 [D1—CH_2—CH_2—CO_2H]

RN 27121-71-7 CAPLUS
CN 21H,23H-Porphine-C,C,C,2-tetrapropanoic acid, C,C,C,3-tetramethyl- (9CI) (CA INDEX NAME)



4 (D1—Me)

4 [D1—CH_2—CH_2—CO_2H]

L7 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:736060 CAPLUS
DOCUMENT NUMBER: 137:242163
TITLE: Method and compositions for optimizing blood and tissue stability of camptothecin and other albumin-binding therapeutic compounds
INVENTOR(S): Burke, Thomas G.; Carter, Daniel C.
PATENT ASSIGNEE(S): New Century Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002074246	A2	20020926	WO 2002-US8301	20020320
WO 2002074246	A3	20030220		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002193318	A1	20021219	US 2002-101513	20020320

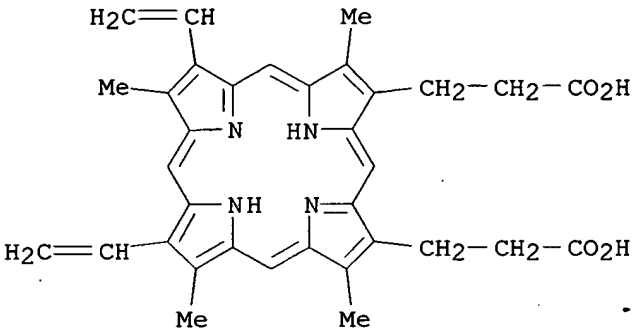
PRIORITY APPLN. INFO.: US 2001-276908P P 20010320

AB The present invention provides methods and formulations for optimizing the anti-cancer and anti-HIV activities of a camptothecin drug, including camptothecin and its related analogs including 9-aminocamptothecin and 9-nitrocamptothecin. The invention involves methodologies and formulations that limit human serum albumin-mediated redn. of the anti-cancer and anti-HIV effects of the camptothecins, and the methods and formulations provide combination therapies in which binding of the

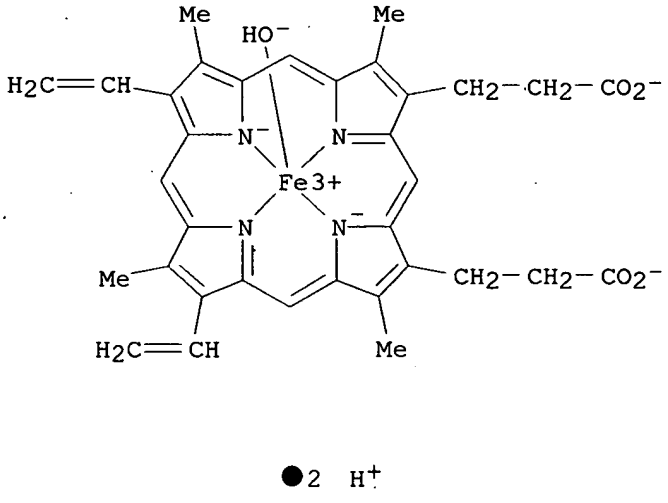
camptothecin agent to human serum albumin can be modulated by the administration of a competing agent that also binds human serum albumin. Reduced camptothecin drug binding to human serum albumin can result in elevated camptothecin free drug levels and thus improve the effectiveness of treatment regimens involving these drugs. Further agents such as methotrexate and AZT can also be used in cancer and HIV-pos. patients employing camptothecin drugs.

IT **553-12-8,** Protoporphyrin **15489-90-4,** Hematin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(optimizing blood and tissue stability of camptothecin and other albumin-binding therapeutic compds.)

RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 15489-90-4 CAPLUS
CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]hydroxy-, dihydrogen, (SP-5-13)- (9CI). (CA INDEX NAME)



● 2 H^+

L7 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:115086 CAPLUS
DOCUMENT NUMBER: 134:178573
TITLE: Process for the metalloporphyrin catalyzed oxidation of organic compounds
INVENTOR(S): Bernardelli, Patrick
PATENT ASSIGNEE(S): Warner Lambert Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809

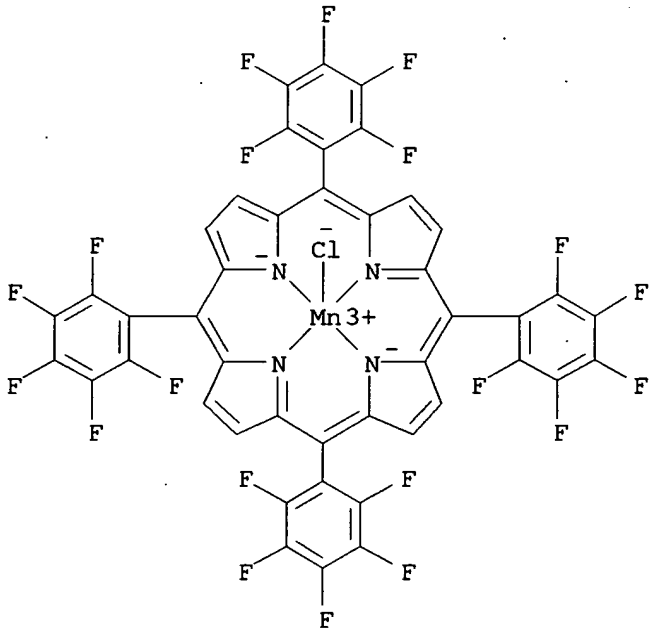
PRIORITY APPLN. INFO.: US 1999-148079P P 19990810
US 1999-150101P P 19990820
WO 2000-EP7726 W 20000809

OTHER SOURCE(S): CASREACT 134:178573

AB An org. compd. (e.g., **Diazepam**) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, aprotic, polyhalogenated solvent (benzotrifluoride). Oxidn. of **diazepam** is conducted to mimic oxidn. (metab.) in biol. systems. The products of the oxidn. of **diazepam** are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert aprotic solvent shows improved oxidn. yields when compared to prior art (e.g., CH3CN-CH2Cl2-water mixts.).

IT **79968-43-7**
RL: CAT (Catalyst use); USES (Uses)
(process for metalloporphyrin-catalyzed oxidn. of org. compds.)

RN 79968-43-7 CAPLUS
CN Manganese, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

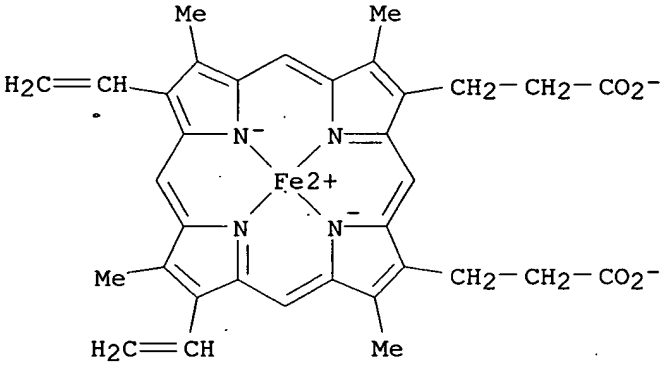
L7 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:141421 CAPLUS
DOCUMENT NUMBER: 131:39882
TITLE: Mechanism-based inhibition of rat liver microsomal **diazepam** C3-hydroxylase by mifepristone associated with loss of spectrally detectable cytochrome P450
AUTHOR(S): Reilly, Paul E. B.; Gomi, Rebecca J.; Mason, Steven R.
CORPORATE SOURCE: Department of Biochemistry, University of Queensland, Brisbane, 4072, Australia
SOURCE: Chemico-Biological Interactions (1999), 118(1), 39-49
CODEN: CBINA8; ISSN: 0009-2797
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Since initial studies with the steroids norethindrone and ethynylestradiol, reported by White and Muller-Eberhard in 1977 (Biochem. J. 166, 57-64), there has been continuing interest in xenobiotics that bear terminal or sub-terminal acetylenic groups which can cause catalysis-dependent inhibition of CYP monooxygenases assocd. either with loss of prosthetic group heme or protein adduct formation. Mifepristone is a synthetic steroid bearing a propyne substitution on carbon 17 and this suggested to us that it may act as a mechanism-based inhibitor of the CYP isoforms responsible for its metab. In human and rat liver, CYP3A isoforms have been implicated in mifepristone clearance and mifepristone administration to rats has also been shown to induce CYP3A enzymes and the assocd. **diazepam** C3-hydroxylase activity (Cheesman, Mason and Reilly, J. Steroid Biochem. Mol. Biol. 58, 1996, 447-454). With microsomes prepd. from the livers of untreated female rats and others in which **diazepam** C3-hydroxylase has been induced, we show here

that mifepristone can cause catalysis-dependent inhibition of this monooxygenase. In addn., incubation of microsomes with mifepristone in the presence, but not in the absence, of NADPH caused loss of spectrally detectable cytochrome P 450. These results suggest that heme adduct formation may result from mifepristone metab. by CYP3A monooxygenases which undergo self-catalyzed irreversible inactivation with this drug as substrate. Since mifepristone administration in vivo is able also to cause induction of the synthesis of hepatic CYP3A apoprotein, mifepristone may have the potential in human medicine for complex interactions with other co-administered drugs which are also substrates for CYP3A monooxygenases.

IT **14875-96-8**, Heme
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(heme adduct formation may result from mifepristone metab. by CYP3A monooxygenases which undergo self-catalyzed irreversible inactivation with this drug as substrate)

RN 14875-96-8 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H^+

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2003 ACS

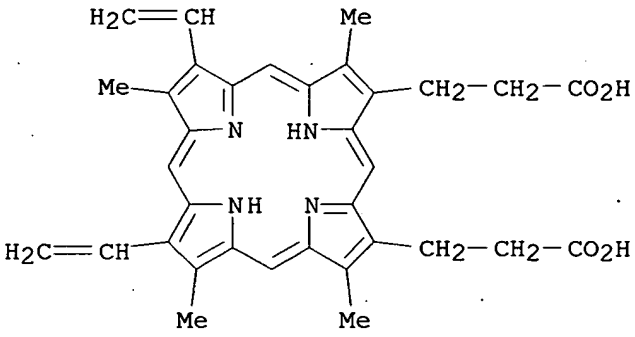
ACCESSION NUMBER: 1998:777319 CAPLUS
DOCUMENT NUMBER: 130:90895
TITLE: Effect of benzodiazepines and neurosteroids on ammonia-induced swelling in cultured astrocytes
AUTHOR(S): Bender, Alex S.; Norenberg, Michael D.
CORPORATE SOURCE: Laboratory of Neuropathology, Veterans Administration Medical Center, Miami, FL, USA
SOURCE: Journal of Neuroscience Research (1998), 54(5), 673-680
CODEN: JNREDK; ISSN: 0360-4012
PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Astroglial swelling occurs in acute hyperammonemic states, including acute hepatic encephalopathy. In these conditions, the peripheral-type benzodiazepine receptor (PBR), a receptor assocd. with neurosteroidogenesis, is up-regulated. This study examd. the potential involvement of PBRs and neurosteroids in ammonia-induced astrocyte swelling in culture. At low micromolar concns., the PBR antagonist PK 11195, atrial natriuretic peptide, and protoporphyrin IX, which are known to interact with the PBR, attenuated (16-100%) the effects of ammonia, whereas the PBR agonists Ro5-4864, **diazepam** binding inhibitor (DBI51-70), and octadecaneuropeptide exacerbated (10-15%) the effects of ammonia. At micromolar concns., **diazepam**, which interacts with both the PBR and the central-type benzodiazepine receptor (CBR), increased swelling by 11%, whereas flumazenil, a CBR antagonist, had no effect. However, at 100 nM **diazepam** and flumazenil abrogated ammonia-induced swelling. The neurosteroids dehydroepiandrosterone sulfate, tetrahydroprogesterone, pregnenolone sulfate, and tetrahydrodeoxycorticosterone (THDOC), products of PBR stimulation, at micromolar concns. significantly enhanced (70%) ammonia-induced swelling. However, at nanomolar concns., these neurosteroids, with exception of THDOC, blocked ammonia-induced swelling. The authors conclude that neurosteroids and agents that interact with the PBR influence ammonia-induced swelling. These agents may represent novel therapies for acute hyperammonemic syndromes and other conditions assocd. with brain edema and astrocyte swelling.

IT **553-12-8**, Protoporphyrin IX
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(benzodiazepines and neurosteroids on ammonia-induced swelling in cultured astrocytes)

RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:255694 CAPLUS
DOCUMENT NUMBER: 129:23391

TITLE: Evidence for the existence of [3H]-trimetazidine binding sites involved in the regulation of the mitochondrial permeability transition pore

AUTHOR(S): Morin, Didier; Elimadi, Aziz; Sapena, Rosa; Crevat, Aime; Carrupt, Pierre-Alain; Testa, Bernard; Tillement, Jean-Paul

CORPORATE SOURCE: Departement de Pharmacologie, IM3, Faculte de Medecine de Paris XII, Creteil, F-94010, Fr.

SOURCE: British Journal of Pharmacology (1998), 123(7), 1385-1394
CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Stockton Press

DOCUMENT TYPE: Journal

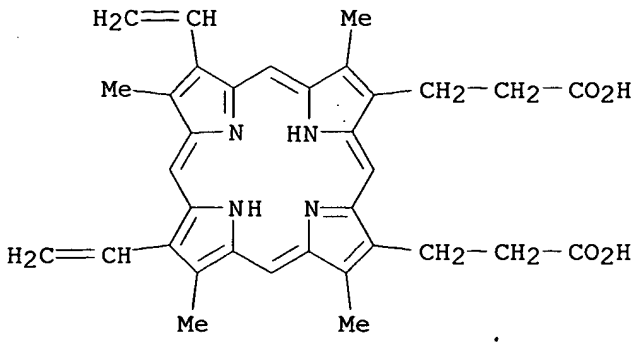
LANGUAGE: English

AB Trimetazidine is an anti-ischemic drug effective in different exptl. models but its mechanism of action is not fully understood. Data indicate that mitochondria could be the main target of this drug. The aim of this work was to investigate the binding of [3H]-trimetazidine on a purified prepn. of rat liver mitochondria. [3H]-trimetazidine binds to two populations of mitochondrial binding sites with Kd values of 0.96 and 84 .mu.M. The total concn. of binding sites is 113 pmol mg-1 protein. Trimetazidine binding sites are differently distributed. The high-affinity ones are located on the outer membranes and represent only a small part (4%) of total binding sites, whereas the low-affinity ones are located on the inner membranes and are more abundant (96%) with a Bmax = 108 pmol mg-1 protein. Drug displacement studies with pharmacol. markers for different mitochondrial targets showed that [3H]-trimetazidine binding sites are different from previously described mitochondrial sites. The possible involvement of [3H]-trimetazidine binding sites in the regulation of the mitochondrial permeability transition pore (MTP), a voltage-dependent channel sensitive to cyclosporin A, was investigated with mitochondrial swelling expts. Trimetazidine inhibited the mitochondrial swelling induced by Ca2+ plus tert-butylhydroperoxide (t-BH). This effect was concn.-dependent with an IC50 value of 200 .mu.M. Assuming that trimetazidine effectiveness may be related to its structure as an amphiphilic cation, the authors compared it with other compds. exhibiting the same chem. characteristic both for their ability to inhibit MTP opening and to displace [3H]-trimetazidine bound to mitochondria. Selected compds. were drugs known to interact with various biol. membranes. A strong correlation between swelling inhibition potency and low-affinity [3H]-trimetazidine binding sites was obsd.: r=0.907. These data suggest that mitochondrial sites labeled with [3H]-trimetazidine may be involved in the MTP inhibition.

IT **553-12-8**, Protoporphyrin IX
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(evidence for existence of [3H]-trimetazidine binding sites involved in regulation of mitochondrial permeability transition pore and effect of other agents in relation to anti-ischemic activity)

RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)

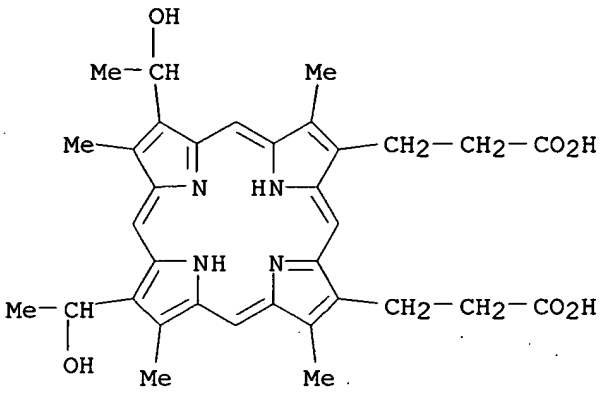


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:470374 CAPLUS
DOCUMENT NUMBER: 127:171391
TITLE: The relaxant effect of **diazepam** on rat tracheal strips
AUTHOR(S): Fehri, Badreddine; Advenier, Charles
CORPORATE SOURCE: Department de Pharmacologie et de Toxicologie, Societe des Industries Pharmaceutiques de Tunisie, Ben Arous, Tunisia
SOURCE: Journal de Pharmacie de Belgique (1997), 52(3), 117-122
CODEN: JPBEAJ; ISSN: 0047-2166
PUBLISHER: Masson
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of **diazepam** was studied on the rat isolated trachea pre-contracted with acetylcholine 10-3 M. **Diazepam** induced a dose-dependent relaxant effect, with EC50 values 2.02 .+-. 0.28 x 10-4 M in controls (n=38). The effect of **diazepam** was not modified by flumazenil (10-6 to 10-4 M) or RP 52028 (10-6 to 10-4 M), which are antagonists of central and peripheral benzodiazepine receptors, resp. No antagonism was obsd. between **diazepam** and nucleotides or endogenous ligands (adenosine 10-6 to 10-4 M, UTP 10-6 to 10-4 M, hematoporphyrin 10-5 and 10-4 M or nicotinamide 10-5 and 10-4 M). These results excluded an endogenous ligand-mediated interaction between nucleotides and **diazepam**. Propranolol (10-7 M) did not modify the **diazepam**-induced relaxation, which excluded an involvement of .beta. receptors in **diazepam** relaxation. Theophylline (10-7 and 10-6 M), IBMX (10-5 and 10-4 M) rolipram (10-5 and 10-4 M) and siguazodan (10-6 to 10-4 M) displayed to the left the concn.-response curves to **diazepam**. The adenyl cyclase activator forskolin (10-7 to 10-5 M), the .beta.-adrenoceptor stimulant isoprenaline (3 x 10-5 M) and the direct acting G-protein stimulant NaF (10-3 M) also produced a leftward shift in the **diazepam** concn.-response curve. The relaxant concn.-effect curves to isoprenaline and to sodium nitroprusside were shifted to the left in a concn.-related manner by **diazepam**. **Diazepam** was more potent on the isoprenaline than on nitroprusside-induced relaxation. These results suggest that the **diazepam**-induced relaxation in the rat isolated trachea is mediated by an inhibition of cyclic nucleotide phosphodiesterases.

IT **14459-29-1**, Hematoporphyrin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(**diazepam** relaxant effect on tracheal strips, and relation to benzodiazepine binding sites and adenylate cyclase system)
RN 14459-29-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)

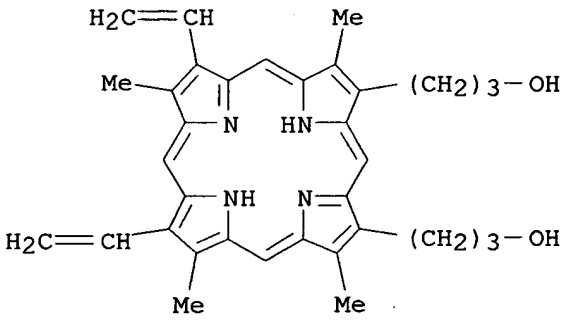


L7 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:248410 CAPLUS
DOCUMENT NUMBER: 126:324937
TITLE: Hemin-induced erythroid differentiation of human myeloleukemia K562 cell line and its modification by bioresponse modifiers
AUTHOR(S): Nakajima, Osamu; Iwasaki, Shigeo; Hashimoto, Yuichi
CORPORATE SOURCE: Institute Molecular Cellular Biosciences, University Tokyo, Tokyo, 113, Japan
SOURCE: Cellular and Molecular Biology (Paris) (1997), 43(1), 115-134
CODEN: CMOBEF; ISSN: 0145-5680
PUBLISHER: C.M.B. Association
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have found that protoporphyrin IX, which had been regarded as inactive, induces erythroid differentiation. The differentiation-inducing activities of various hemin-related compds., including hematoporphyrin IX, mesoporphyrin IX, deuteroporphyrin IX and protoporphyrin IX di-Me ester, suggested certain structural requirements for the activity: (1) the iron moiety of hemin is not essential, and (2) the propionic acid side chains of hemin play an important role. In addn., we have examd. the influence of some bioactive factors on hemin/protoporphyrin IX-induced differentiation of K562 cell line. Retinoids and tubulin-disruptors dose-dependently enhanced hemin/protoporphyrin IX-induced differentiation of K562 cells, though they did not themselves induce differentiation. Retinoid antagonists suppressed hemin-induced differentiation. The effects of hemin and/or retinoids on the mRNA expressions of oncogenes (c-myc and c-myb) and retinoic acid receptor genes (rar .alpha. and rar .beta.) of K562 cells were analyzed. We also examd. the possible

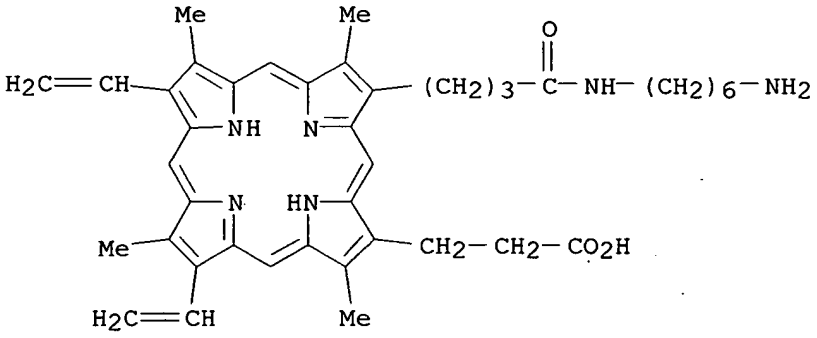
involvement of peripheral-type benzodiazepine receptor (PBR) in hemin/protoporphyrin IX-induced differentiation of K562 cells by the use of its ligands. **Diazepam** itself was revealed to possess differentiation-inducing activity on K562 cells. The PBR-specific ligands modified hemin-induced differentiation. These results suggest a requirement for retinoids (or retinoid-like cofactors) for hemin/protoporphyrin IX-induced differentiation of K562 cells and the involvement of PBR in erythroid differentiation of K562 cell line.

IT **76915-39-4P 189622-00-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relations of hemin-induced erythroid differentiation of human myeloleukemia K562 cell line and its modification by bioresponse modifiers)

RN 76915-39-4 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanol, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



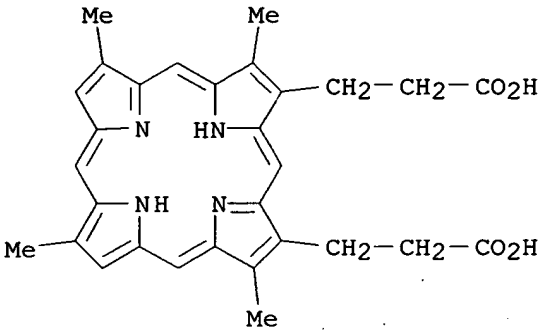
RN 189622-00-2 CAPLUS
CN 21H,23H-Porphine-2-propanoic acid, 18-[4-[(6-aminohexyl)amino]-4-oxobutyl]-7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



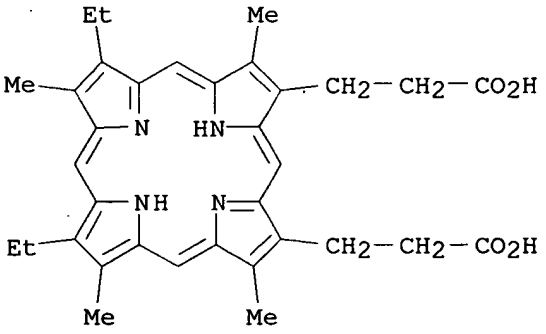
IT **448-65-7**, Deuteroporphyrin IX **493-90-3**, Mesoporphyrin IX **531-14-6**, Coproporphyrin I **5522-63-4**, Coproporphyrin III tetramethyl ester **14325-05-4 14459-29-1**, Hematoporphyrin IX **15442-64-5**, Zinc protoporphyrin IX **16009-13-5 73170-32-8 79236-56-9**

106283-63-0 153760-87-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relations of hemin-induced erythroid differentiation of human myeloleukemia K562 cell line and its modification by bioresponse modifiers)

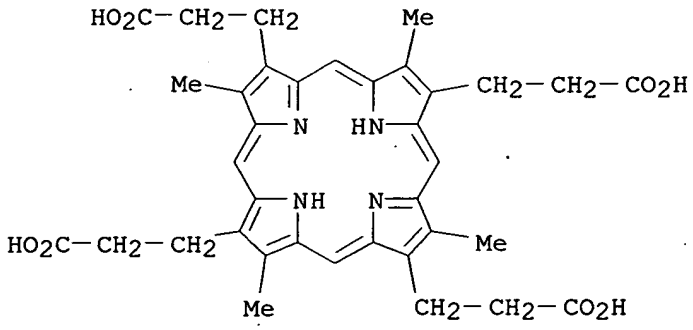
RN 448-65-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- (9CI) (CA INDEX NAME)



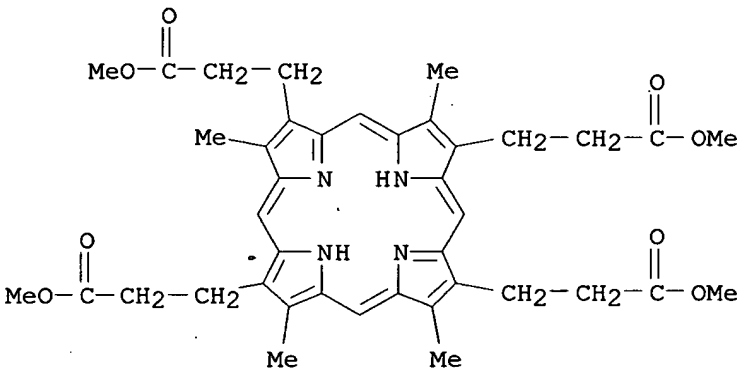
RN 493-90-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



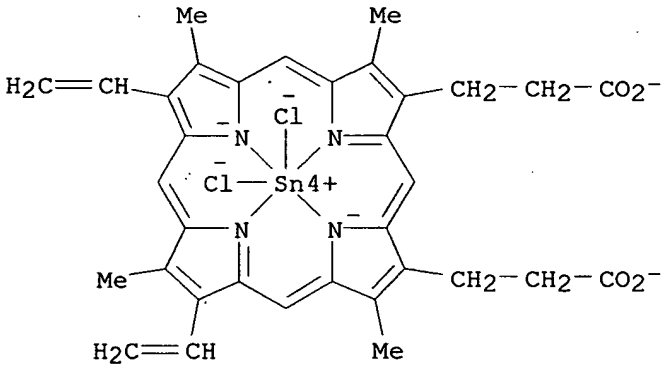
RN 531-14-6 CAPLUS
CN 21H,23H-Porphine-2,7,12,17-tetrapropanoic acid, 3,8,13,18-tetramethyl- (9CI) (CA INDEX NAME)



RN 5522-63-4 CAPLUS
CN 21H,23H-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetramethyl-, tetramethyl ester (9CI) (CA INDEX NAME)

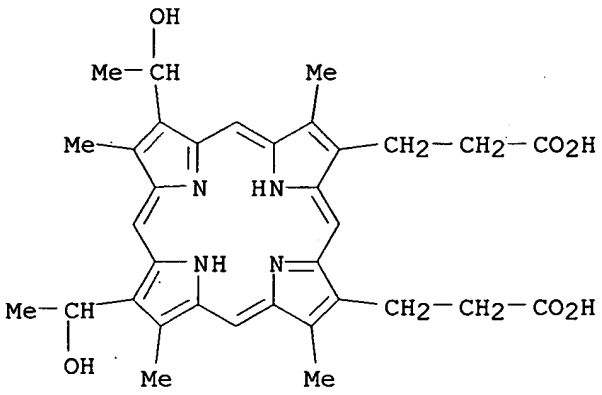


RN 14325-05-4 CAPLUS
CN Stannate(2-), dichloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (OC-6-13)- (9CI) (CA INDEX NAME)

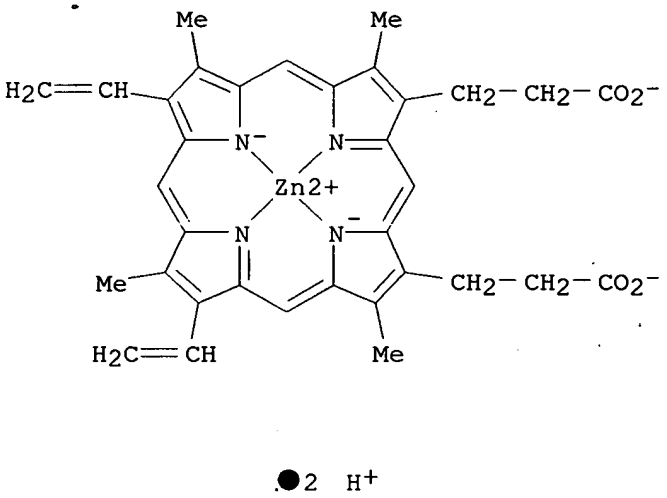


2 H^+

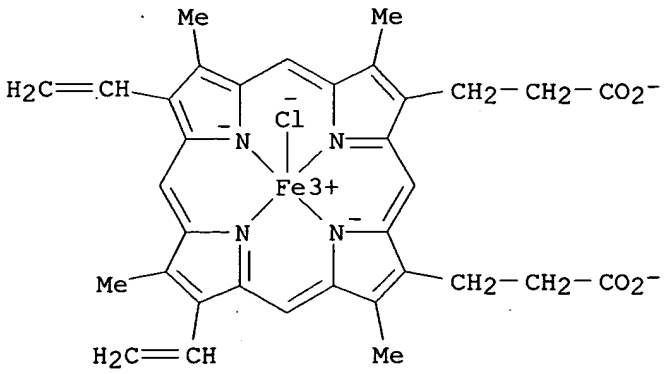
RN 14459-29-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 15442-64-5 CAPLUS
CN Zincate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)

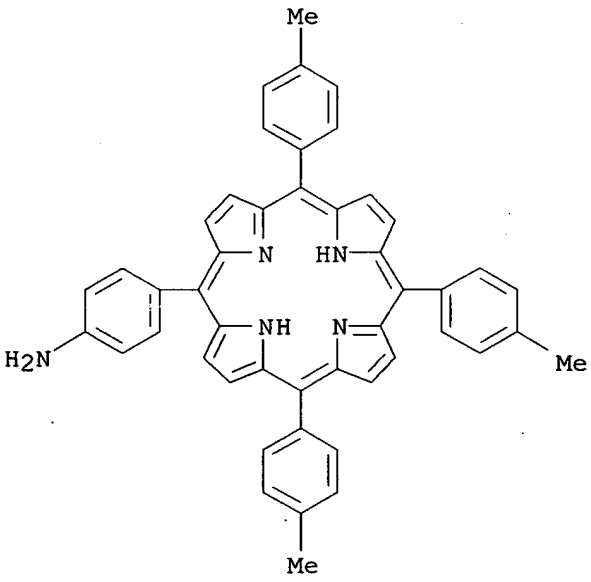


RN 16009-13-5 CAPLUS
CN Ferrate(2-), chloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)

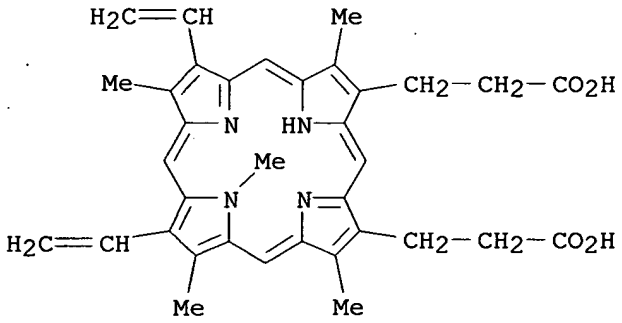


●2 H^+

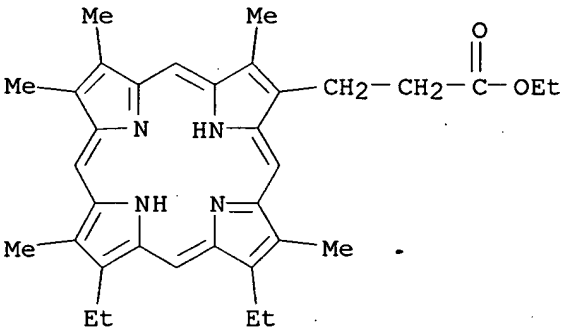
RN 73170-32-8 CAPLUS
CN Benzenamine, 4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)



RN 79236-56-9 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17,23-pentamethyl- (9CI) (CA INDEX NAME)

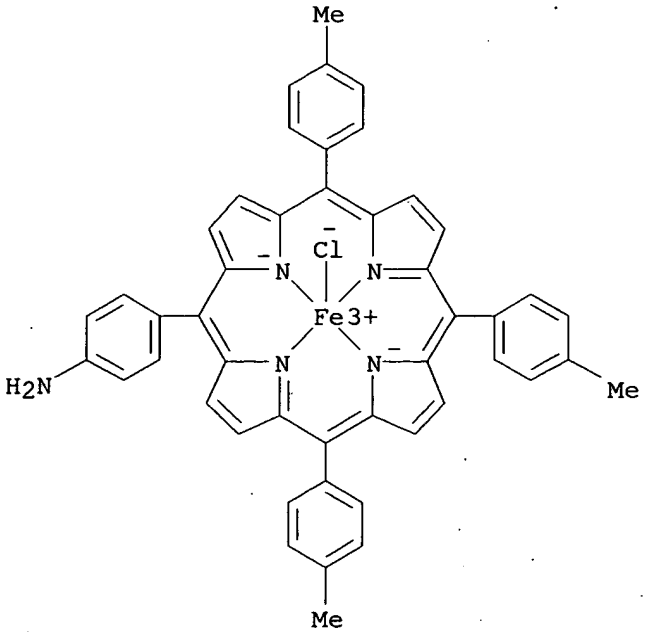


RN 106283-63-0 CAPLUS
CN 21H,23H-Porphine-2-propanoic acid, 13,17-diethyl-3,7,8,12,18-pentamethyl-, ethyl ester (9CI) (CA INDEX NAME)

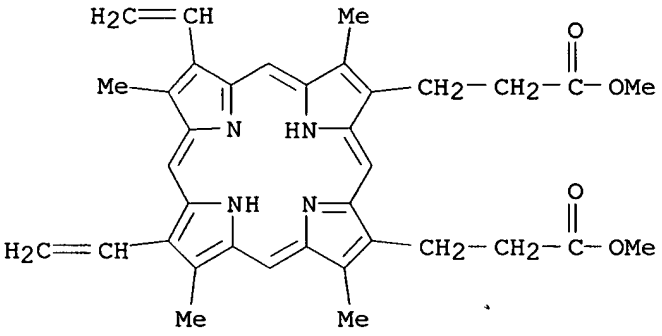


RN 153760-87-3 CAPLUS
CN Iron, chloro[5-(4-aminophenyl)-10,15,20-tris(4-methylphenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-13)-(9CI) (CA INDEX NAME)

o

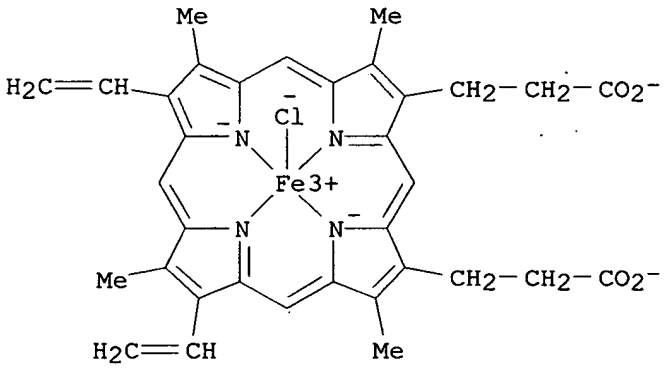


IT **5522-66-7,** Protoporphyrin IX dimethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(structure-activity relations of hemin-induced erythroid differentiation of human myeloleukemia K562 cell line and its modification by bioresponse modifiers)
RN 5522-66-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:75960 CAPLUS
DOCUMENT NUMBER: 126:166810
TITLE: The response of IL-3 dependent B6SUtA bone marrow cells to both erythropoietin and chemical inducers of differentiation
AUTHOR(S): Ishiguro, Kimiko; C. Sartorelli, Alan
CORPORATE SOURCE: Department of Pharmacology and Developmental

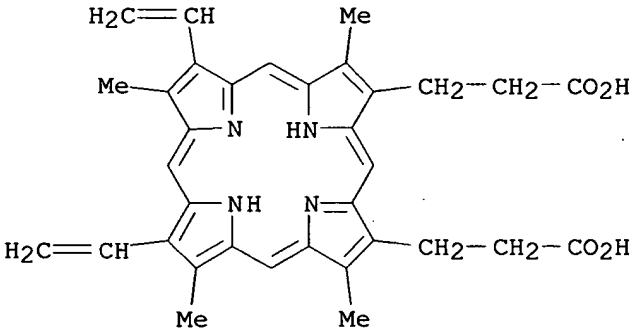
Therapeutics Program, Cancer Center, Yale University School of Medicine, 333 Cedar Street, New Haven, CT, 06520, USA
SOURCE: Cancer Letters (Shannon, Ireland) (1996), 110(1,2), 233-241
CODEN: CALEDQ; ISSN: 0304-3835
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To develop cell lines which respond to both a physiol. cytokine and chem. agents by the induction of differentiation pathway, factor dependent B6SUtA murine bone marrow cells were transfected with the erythropoietin receptor (EpoR). Clones were obtained that exhibited different sensitivities to erythropoietin (Epo), with one clone exhibiting erythroid differentiation in response to Epo, while in another Epo acted as a proliferation stimulus. Moreover, parental B6SUtA cells were sensitive to the initiation of differentiation by butyrate, **diazepam** and hemin. Thus, B6SUtA cells appear to represent a unique model to dissect the signaling mols. involved in the growth and differentiation pathways employed by Epo and nonphysiol. chems.
IT **16009-13-5**, Hemin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(B6SUtA bone marrow erythropoietin receptor-transfected cell response to erythropoietin and chem. inducers of differentiation)
RN 16009-13-5 CAPLUS
CN Ferrate(2-), chloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)



●2 H^+

L7 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:584859 CAPLUS
DOCUMENT NUMBER: 125:272485
TITLE: PK 11195 aggravates 3,5-diethoxycarbonyl-1,4-dihydrocollidine-induced hepatic porphyria in rats
AUTHOR(S): Fonia, Ora; Weizman, Ronit; Coleman, Raymond;

Kaganovskaya, Ella; Gavish, Moshe
CORPORATE SOURCE: Department Pharmacology, Bruce Rappaport Faculty Medicine, Haifa, 31096, Israel
SOURCE: Hepatology (Philadelphia) (1996), 24(3), 697-701
CODEN: HPTLD9; ISSN: 0270-9139
PUBLISHER: Saunders
DOCUMENT TYPE: Journal
LANGUAGE: English
AB There is evidence to suggest that peripheral-type benzodiazepine receptors (PBR) are involved in porphyrin transport during erythroid differentiation, and it is possible that these receptors have an important role in heme biosynthesis. The authors examd. the biochem. and ultrastructural alterations in rat liver following exptl. induced acute hepatic porphyria, as well as the effects of the administration of a selective PBR ligand, PK 11195. The most severe pathol. conditions were found in rats that received a combined treatment of the porphyrinogenic agent 3,5-diethoxycarbonyl-1,4-dihydrocollidine (DDC) and PK 11195. TEM showed a correlation between the ultrastructural pathol. of the liver, the total porphyrin levels in urine and liver, and the porphobilinogen levels in urine. Hepatocytes in this acute porphyria showed the development of large secondary lysosomes contg. cryst. aggregates of protoporphyrin. Bile canaliculi were grossly enlarged, contained aggregates of protoporphyrin crystals, and showed the presence of bile thrombi. In addn., prominent bundles of collagen fibers (fibrosis) were commonly found in livers of rats that had been treated with DDC or DDC and PK 11195. The authors conclude that the administration of PK 11195 to porphyric rats aggravates porphyrin accumulation and cellular damage in the liver. Perhaps this evidence suggests that PK 11195 blocks the binding of protoporphyrin IX to PBR thus elevating the content of protoporphyrin IX in liver.
IT **553-12-8**, Protoporphyrin IX
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(ligand for peripheral-type benzodiazepine receptors aggravates hepatic porphyria and liver accumulation of)
RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



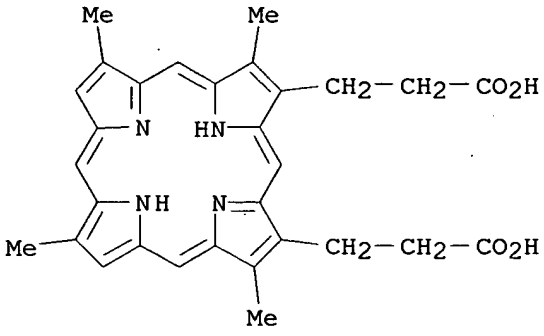
L7 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:730333 CAPLUS
DOCUMENT NUMBER: 123:160249

TITLE: Possible involvement of peripheral-type benzodiazepine receptors in erythroid differentiation of human leukemia cell line, K562
AUTHOR(S): Nakajima, Osamu; Hashimoto, Yuichi; Iwasaki, Shigeo
CORPORATE SOURCE: Inst. Mol. Cell. Biosci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Biological & Pharmaceutical Bulletin (1995), 18(6), 903-6
CODEN: BPBLEO; ISSN: 0918-6158
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

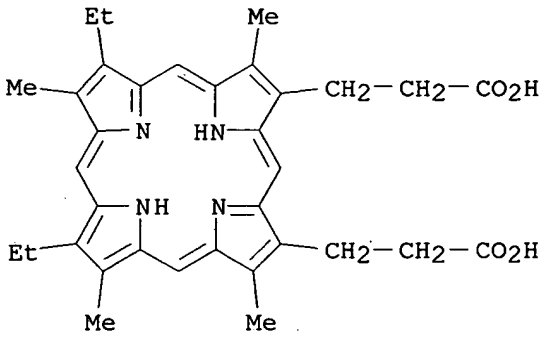
AB Possible involvement of the peripheral-type benzodiazepine receptor (PBR) in hemin/protoporphyrin-induced erythroid differentiation of human leukemia K562 cells was investigated by the use of the ligands, **diazepam** and PK11195. **Diazepam** itself exhibited differentiation-inducing activity on K562 cells. The PBR-specific antagonist, PK11195, dose-dependently inhibited both **diazepam** -induced and hemin/protoporphyrin-induced K562 cell differentiation. The results imply that PBR is involved in the erythroid differentiation of K562 cells.

IT **448-65-7**, Deuteroporphyrin **493-90-3**, Mesoporphyrin **553-12-8**, Protoporphyrin IX **14459-29-1**, Hematoporphyrin **16009-13-5**, Hemin **27121-71-7**, Coproporphyrin **79236-56-9**, N-Methylprotoporphyrin IX
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(possible involvement of peripheral-type benzodiazepine receptors in hemin/protoporphyrin-induced erythroid differentiation of human leukemia cell line K562)

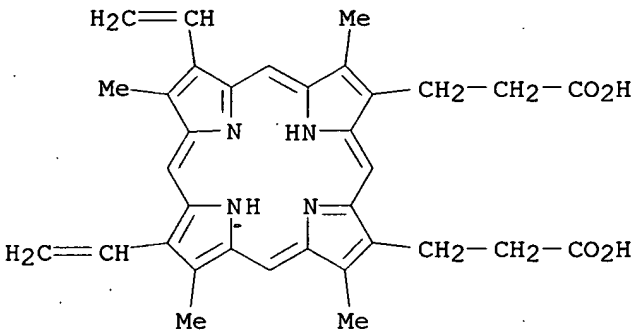
RN 448-65-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- (9CI) (CA INDEX NAME)



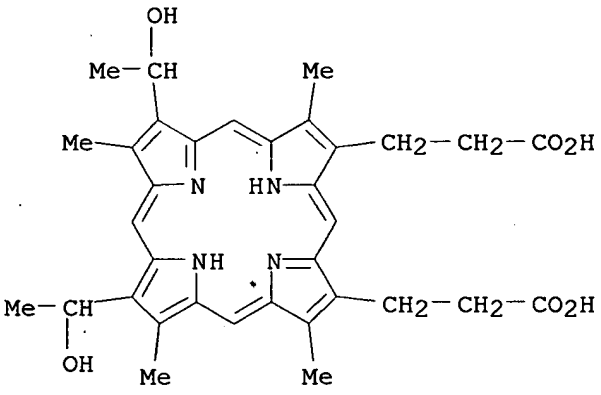
RN 493-90-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)

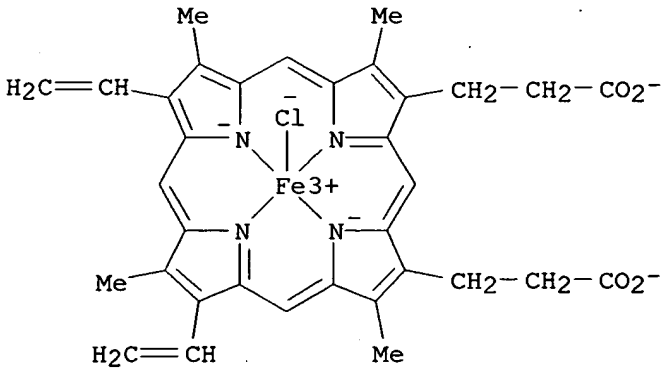


RN 14459-29-1 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



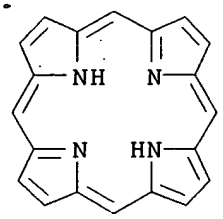
RN 16009-13-5 CAPLUS
CN Ferrate(2-), chloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-,

dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)



●2 H^+

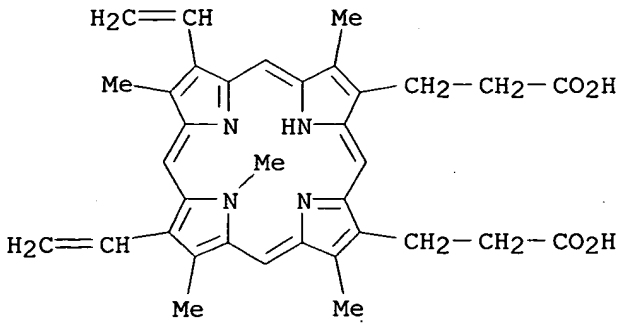
RN 27121-71-7 CAPLUS
CN 21H,23H-Porphine-C,C,C,2-tetrapropanoic acid, C,C,C,3-tetramethyl- (9CI) (CA INDEX NAME)



4 (D1—Me)

4 [D1—CH_2—CH_2—CO_2H]

RN 79236-56-9 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17,23-pentamethyl- (9CI) (CA INDEX NAME)

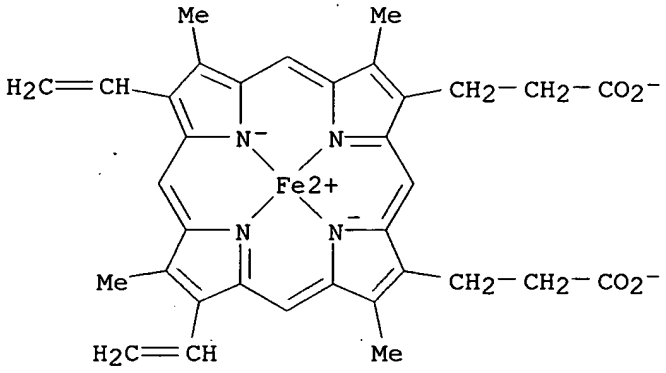


L7 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:598322 CAPLUS
DOCUMENT NUMBER: 123:6645
TITLE: Involvement of peripheral-type benzodiazepine receptors in the intracellular transport of heme and porphyrins
AUTHOR(S): Taketani, Shigeru; Kohno, Hirao; Furukawa, Takako; Tokunaga, Rikio
CORPORATE SOURCE: Dep. Hygiene, Kansai Medical Univ., Osaka, 570, Japan
SOURCE: Journal of Biochemistry (Tokyo) (1995), 117(4), 875-80
CODEN: JOBIAO; ISSN: 0021-924X
PUBLISHER: Japanese Biochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To investigate the involvement of peripheral-type benzodiazepine receptors (PBR) in heme metab., we examd. the interaction of [55Fe] heme with PBR. Transfection of the cloned mouse PBR-isoquinoline carboxamide-binding protein (PBR/IBP) cDNA into monkey kidney Cos-1 cells resulted in a 2.5-fold increase in [55Fe]hemin binding sites, concomitant with the increase in [3H]PK11195 binding sites, as compared with those seen in antisense PBR/IBP cDNA-transfected cells. The binding of hemin to the transfected receptors exhibited a relatively high affinity with a Kd of 12 nM, and was inhibited by several benzodiazepine ligands, including PK11195, Ro 5-4864, **diazepam** and protoporphyrin IX. When mouse liver mitochondria were incubated with [55Fe]hemin, the binding to PBR had a Kd of 15.+-.1.8 nM. The Bmax of [55Fe]hemin binding to the mitochondria was 6.88.+-.0.76 pmol/mg of protein, a value consistent with that of [3H]PK11195 binding, with a lower affinity. Coproporphyrinogen III, a precursor porphyrin produced in the cytosol, is translocated into mitochondria, then it is converted to protoporphyrinogen IX; this conversion decreased in the presence of benzodiazepine ligands. To examine whether this decrease was related to a decrease in the binding of coproporphyrinogen to the mitochondria, the effects of benzodiazepines on the binding of coproporphyrinogen were examd. As the binding was dose-dependently inhibited by PK11195, Ro 5-4864, and **diazepam**, porphyrins are likely to be endogenous ligands for PBR. We propose that PBR play a role in the intracellular transport of porphyrins and heme.

IT **14875-96-8**, Heme
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(involvement of peripheral-type benzodiazepine receptors in intracellular transport of heme and porphyrins)
RN 14875-96-8 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



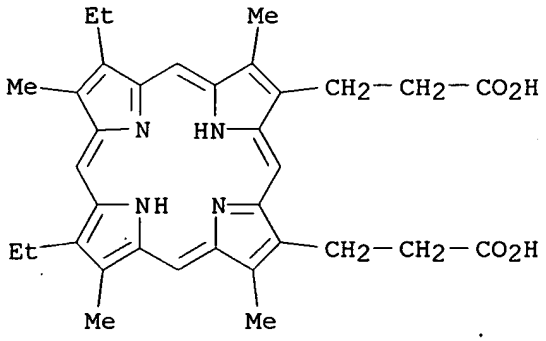
●2 H^+

L7 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:576339 CAPLUS
DOCUMENT NUMBER: 121:176339
TITLE: Characterization of peripheral benzodiazepine receptors in rat prostatic adenocarcinoma
AUTHOR(S): Batra, Satish; Älenfall, Jan
CORPORATE SOURCE: Kabi Pharm. Oncol., Univ. Lund, Lund, S-223 63, Swed.
SOURCE: Prostate (New York, NY, United States) (1994), 24(5), 269-78
CODEN: PRSTDS; ISSN: 0270-4137
DOCUMENT TYPE: Journal
LANGUAGE: English

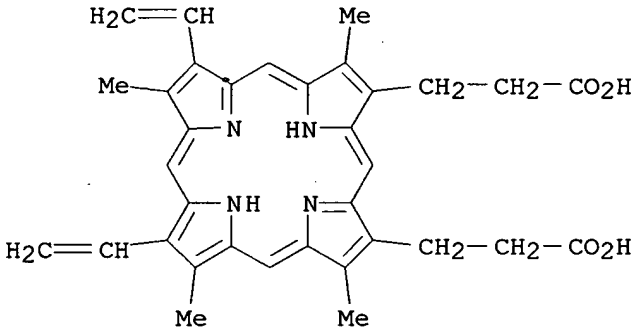
AB By using PK 11195, a high-affinity ligand for peripheral benzodiazepine receptors (PBZr), binding sites in isolated mitochondrial (m-fraction) and microsomal (p-fraction) fractions from R-3327 Dunning AT-1 tumors in rats and from normal rat ventral and dorsolateral prostate were studied. Binding of PK 11195 in both the m- and p-fractions from AT-1 tumors, but only in the m-fraction from the ventral and dorsolateral prostate, was specific, saturable, and of high affinity. The PBZr d. in the m-fraction from AT-1 tumors was 6-fold and 20-fold higher than that in the ventral and dorsolateral prostate, resp. The receptor d. in the p-fraction from AT-1 tumors was approx. 25% of that in the m-fraction. Clear differences were obsd. in the competition by both **diazepam** and flunitrazepam for binding sites in the m- and p-fractions from tumors. These data indicate that the receptors were not only present in the mitochondria, but were also present in considerable amts. in the microsomal fractions. The unusually high amts. of receptors in the fast-growing anaplastic prostatic tumor suggest their involvement in the regulation of cell proliferation and possibly in tumorigenesis.

IT **493-90-3**, Mesoporphyrin **553-12-8**, Protoporphyrin
RL: BIOL (Biological study)
(binding of, to benzodiazepine receptors of prostate adenocarcinoma)

RN 493-90-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



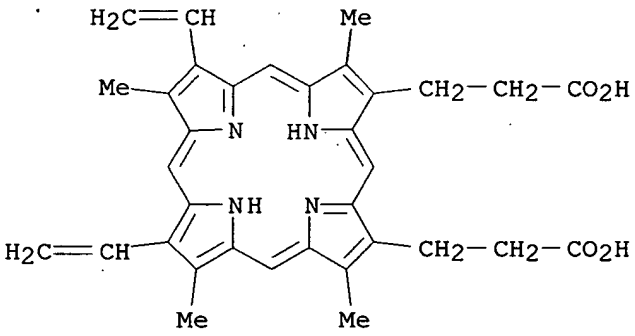
L7 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:450249 CAPLUS
DOCUMENT NUMBER: 121:50249
TITLE: Computer-assisted molecular modeling of benzodiazepine and thyromimetic inhibitors of the HepG2 iodothyronine membrane transporter
AUTHOR(S): Kragie, Laura; Forrester, Maureen L.; Cody, Vivian; McCourt, Mary
CORPORATE SOURCE: Fac. Nat. Sci. Math., State Univ. New York, Buffalo, Amherst, NY, 14260, USA
SOURCE: Molecular Endocrinology (1994), 8(3), 382-91
CODEN: MOENEN; ISSN: 0888-8809
DOCUMENT TYPE: Journal
LANGUAGE: English
AB T3 cellular uptake is inhibited in the presence of benzodiazepines (BZs). The structure-activity relationship of BZ inhibition correlates strongly with halogen substitution of the nonfused Ph ring and indicates that this ring is required for activity. A structure-activity series of

thyromimetic (TH) inhibitors of the HepG2 iodothyronine transporter further point out the crit. importance of the amino group of the alanine side chain, its L-stereo configuration, and the size of the substituents of the inner and outer Ph rings. A third series of compds., reported to interact at related sites, were inactive as HepG2 iodothyronine transport inhibitors, and therefore the potent inhibitors were restricted to the BZ and TH compds. Using both of these BZ and TH structure-activity series along with computer-assisted mol. modeling techniques, the authors detd. which chem. structural components were important at the transporter interaction site. By superimposing structures from active chems., excluding residues from poor inhibitors, and incorporating mol. electropotential data, the authors developed a five-point model of BZ conformational similarity to the endogenous transporter ligand, L-T3: the alkyl substitution at the N1 of the BZ ring seems to stimulate the alanine side chain of T3, and the electroneg. halogen and oxygen atoms of substituents at R3/R7/R2'/R4' of BZ form a pyrimidyl pharmacophore that seems to correspond with the 3-1/5-1/3'-1/4'-OH substituents of T3, resp. These points, suggesting a tilted cross-bow formation, may be sites for ligand interaction with the iodothyronine transporter.

IT **553-12-8**
RL: BIOL (Biological study)
(triiodothyronine binding by iodothyronine transporter inhibition by, structure in relation to)

RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1994:405814 CAPLUS

DOCUMENT NUMBER: 121:5814

TITLE: Induction of peripheral-type benzodiazepine receptors during differentiation of mouse erythroleukemia cells. A possible involvement of these receptors in heme biosynthesis

AUTHOR(S): Taketani, Shigeru; Kohno, Hirao; Okuda, Masahiro; Furukawa, Takako; Tokunaga, Rikio

CORPORATE SOURCE: Dep. Hyg., Kansai Med. Univ., Moriguchi, 570, Japan

SOURCE: Journal of Biological Chemistry (1994), 269(10), 7527-31
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

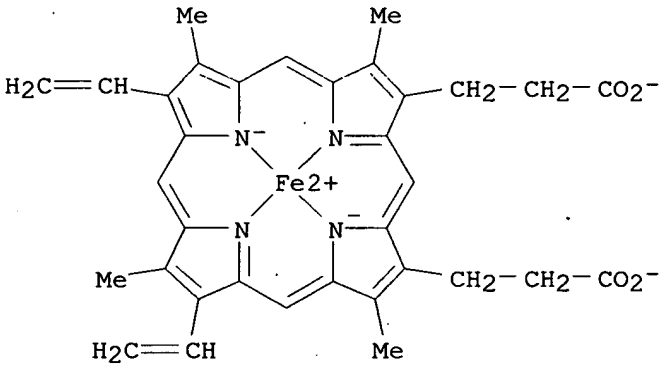
LANGUAGE: English

AB To search for a possible role for peripheral-type benzodiazepine receptors (PBR) during erythroid differentiation, the PBR isoquinoline carboxamide-binding protein (PBR/IBP), an 18-kDa protein on PBR, was cloned from a mouse erythroleukemia (MEL) cell cDNA library. Sequence anal. revealed that PBR/IBP comprises 169 amino acid residues (Mr 18,828), and has a high homol. with PBR/IBP from other sources. The cDNA allows for the expression of active PBR/IBP, exhibiting a high affinity for isoquinoline carboxamide, [3H]PK11195, with Kd of 0.80 and 1.56 nM. RNA blot anal. revealed that treatment of MEL cells with DMSO led to an increase in PBR/IBP mRNA for up to 72 h, with a concomitant induction of mRNAs for heme biosynthetic enzymes, coproporphyrinogen oxidase and ferrochelatase. The induction of PBR/IBP mRNA was also obsd. in MEL cells induced with **diazepam**. The binding activity of [3H]PK11195 in MEL cells showed a high affinity with Kd of 0.69-2.13 nM, and increased during erythroid differentiation. The order of potency of different ligands to compete against [3H]PK11195 binding in induced MEL cells was PK11195 > protoporphyrin IX > **diazepam** > coproporphyrinogen III > coproporphyrin III > estazolam. In contrast to the induction of PBR/IBP in induced MEL cells, the voltage-dependent anion channel (mitochondrial porin) assocd. with PBR remained unchanged. These results suggest that PBR/IBP on PBR may be involved in porphyrin transport and may even be a crit. factor in erythroid-specific induction of heme biosynthesis.

IT **14875-96-8**, Heme
RL: FORM (Formation, nonpreparative)
(formation of, peripheral-type benzodiazepine receptor role in)

RN 14875-96-8 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



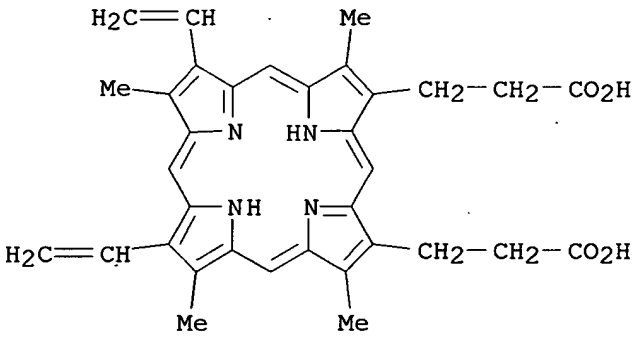
●2 H+

IT **553-12-8 14643-66-4**, Coproporphyrin III
RL: BIOL (Biological study)
(peripheral-type benzodiazepine receptor binding specificity for, in mouse erythroleukemia cells)

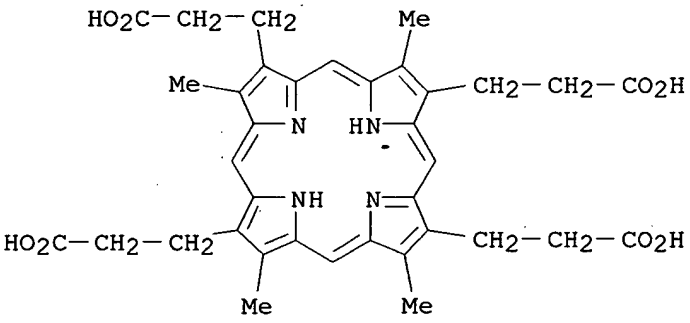
RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-

tetramethyl- (9CI) (CA INDEX NAME)



RN 14643-66-4 CAPLUS
CN 21H,23H-Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



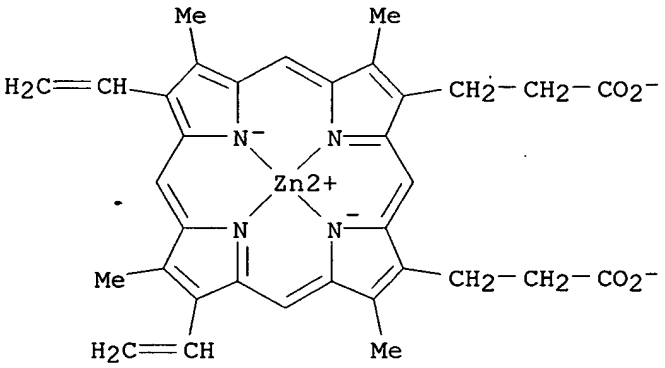
L7 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:76398 CAPLUS
DOCUMENT NUMBER: 118:76398
TITLE: Washing erythrocytes to remove interferents in measurements of zinc protoporphyrin by front-face hematofluorometry
AUTHOR(S): Hastka, J.; Lasserre, J. J.; Schwarzbeck, A.; Strauch, M.; Hehlmann, R.
CORPORATE SOURCE: III Med. Klin., Univ. Heidelberg, Mannheim, 6800/31, Germany
SOURCE: Clinical Chemistry (Washington, DC, United States) (1992), 38(11), 2184-9
CODEN: CLCHAU; ISSN: 0009-9147
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Zinc protoporphyrin (ZPP) is detd. by hematofluorometry of whole blood to detect iron deficiency in blood donors. In hospitalized patients, ZPP did not correlate with established markers of iron status. 4500 ZPP measurements were performed with the Aviv front-face hematofluorometer in samples from 475 patients and ferritin, transferrin satn., Hb, and erythrocyte indexes were measured. The fluorometric detn. is affected by

substances dissolved in plasma but this interference can be eliminated by using washed erythrocytes. In validation tests the within-day variation was <3.5%; the day-to-day variation was <6.8%. In 130 healthy persons without iron deficiency, ZPP was .ltoreq.40 .mu.mol/mol heme, which is considered a normal value. Mean ZPP in 46 iron-deficient patients was 256 (SD 105) .mu.mol/mol heme (correlation with ferritin: -0.73; with Hb: -0.85; P <0.001). When washed erythrocytes are used, the hematofluorometric detn. of ZPP is sensitive and specific for detecting iron deficiency in otherwise healthy individuals and hospitalized patients.

IT **15442-64-5**, Zinc protoporphyrin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in blood of human by front-face hematofluorometry, washing erythrocytes to remove interferents in)

RN 15442-64-5 CAPLUS

CN Zincate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H^+

L7 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1992:420403 CAPLUS

DOCUMENT NUMBER: 117:20403

TITLE: Specific binding sites for [3H]Ro 5-4864 in rat prostate and seminal vesicle

AUTHOR(S): Camins, Antonio; Sureda, Francesc X.; Camarasa, Jorge; Escubedo, Elena

CORPORATE SOURCE: Fac. Pharm., Univ. Barcelona, Barcelona, 08028, Spain

SOURCE: General Pharmacology (1992), 23(3), 381-4
CODEN: GEPHDP; ISSN: 0306-3623

DOCUMENT TYPE: Journal

LANGUAGE: English

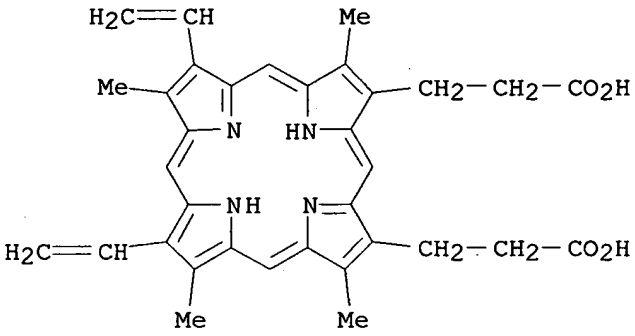
AB The peripheral-type benzodiazepine receptor was characterized in rat prostate and seminal vesicle using [3H]Ro 5-4864 as radioligand. The affinity of this radioligand for this receptor was higher in rat prostate (KD = 4.36 nM) than in seminal vesicle (KD = 8.45 nM). The d. of binding sites obtained in these two tissues was Bmax = 4164 fmol/mg in prostate

and 5978 fmol/mg in seminal vesicle. The [3H]Ro 5-4864 binding was inhibited non-competitively by atractyloside and .alpha.,.beta.-methylene ATP, suggesting a modulation by the ADP/ATP mitochondrial carrier. Flutamide was able to displace bound [3H]Ro 5-4864 with an IC50 similar to protoporphyrin IX.

IT **553-12-8**, Protoporphyrin IX
RL: BIOL (Biological study)
(Ro 5-4864 binding to peripheral benzodiazepine receptors inhibition by, in lab. animal prostate and seminal vesicle)

RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:193119 CAPLUS

DOCUMENT NUMBER: 112:193119

TITLE: Molecular cloning and expression of cDNA encoding a peripheral-type benzodiazepine receptor

AUTHOR(S): Sprengel, Rolf; Werner, Pia; Seeburg, Peter H.; Mukhin, Alexey G.; Santi, M. Rita; Grayson, Dennis R.; Guidotti, Alessandro; Krueger, Karl E.

CORPORATE SOURCE: Zent. Mol. Biol., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Journal of Biological Chemistry (1989), 264(34), 20415-21
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal

LANGUAGE: English

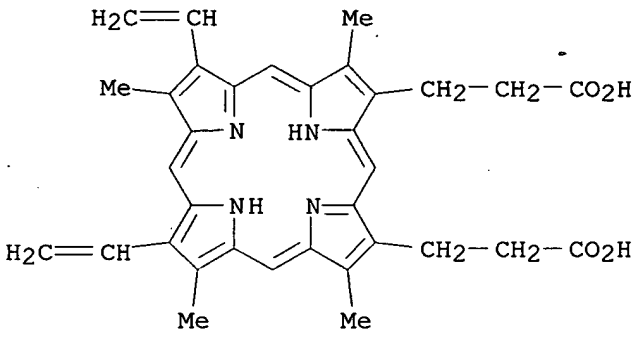
AB This report describes the cloning of a full length cDNA of rat encoding PKBS, a protein of approx. 17 kDa assocd. with peripheral-type benzodiazepine binding sites. Cyanogen bromide digestion of purified PKBS yielded several peptide fragments which were subjected to gas-phase sequencing. Based on these partial amino acid sequences, oligonucleotide probes were used to screen a rat adrenal cDNA library. Several hybridizing clones were isolated which were found to contain overlapping sequences. The longest cDNA spanned 781 base pairs and specified an open reading frame of 169 amino acids which matched all of the peptide sequences. Northern anal. with this PKBS cDNA probe in different rat tissues revealed one RNA species of approx. 850 nucleotides exhibiting relative abundances qual. comparable with the densities of peripheral-type benzodiazepine binding sites in each tissue. The PKBS cDNA was cloned

into an eukaryotic expression vector placing it under transcriptional control of the .beta.-globin promoter and SV40 enhancer. Transfection of the transformed human kidney 293 cell line with this recombinant vector resulted in stoichiometric increases of about 900 fmol/mg of protein in binding capacities for Ro5-4864 (4'-chlorodiazepam) and PK 11195, two peripheral-type benzodiazepine ligands. These increases were accounted for by the expression of binding sites with approx. dissocn. consts. of 5 nM for PK 11195 and 8 nM for Ro5-4864, thereby distinguishing the expressed binding sites as being characteristic of the receptor from rat origin rather than of the host human-derived cell line. The rank order of potency of different ligands to compete against [3H]Ro5-4864 binding in the transfected cells was PK 11195 > Ro5-4864 > **diazepam** > protoporphyrin IX > clonazepam, consistent with the specificity characteristic of rat peripheral type benzodiazepine binding sites. These studies suggest that PKBS comprises binding domains for benzodiazepines and isoquinoline carboxamides and hence is apparently responsible for the manifestation of peripheral-type benzodiazepine recognition sites.

IT **553-12-8**, Protoporphyrin IX
RL: PRP (Properties)
(protein PKBS of rat binding to, cDNA for, cloning and expression of)

RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1990:151779 CAPLUS

DOCUMENT NUMBER: 112:151779

TITLE: Peripheral type benzodiazepine receptors in human and guinea pig lung: characterization and autoradiographic mapping

AUTHOR(S): Mak, Judith C. W.; Barnes, Peter J.

CORPORATE SOURCE: Dep. Thorac. Med., Natl. Heart Lung Inst., London, SW3 6LY, UK

SOURCE: Journal of Pharmacology and Experimental Therapeutics (1990), 252(2), 880-5
CODEN: JPETAB; ISSN: 0022-3565

DOCUMENT TYPE: Journal

LANGUAGE: English

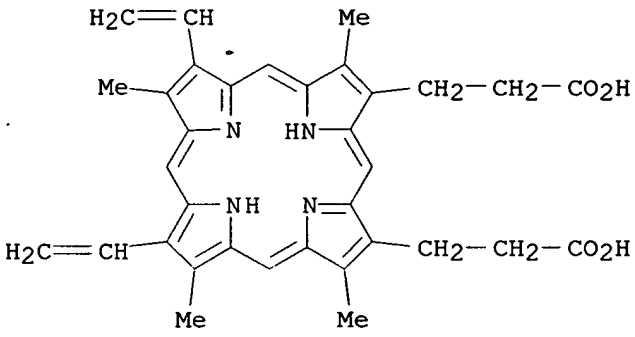
AB Binding of [3H]Ro5-4864, a ligand selective for peripheral-type benzodiazepine receptors, to human and guinea pig lung membranes was characterized and the binding sites localized in lung sections by light

microscopic autoradiog. Inhibition of [3H]Ro5-4864 binding by unlabeled Ro5-4864, PK11195, midazolam, **diazepam**, clonazepam and flumazenil indicated that [3H]Ro5-4864 bound to specific receptors and binding was reversible. Scatchard anal. indicated a single class of binding site, with a dissocn. const. (Kd) of 12.8 nM with max. binding capacity of 2.6 pmol/mg of protein for human lung and Kd of 8.4 nM and max. binding capacity of 3.5 pmol/mg of protein for guinea pig lung. Autoradiograms showed specific labeling over discrete structures in both human and guinea pig lung. Labeling was particularly dense over submucosal glands in intrapulmonary bronchi of human. Airways were also labeled, with epithelium having a higher grain d. than smooth muscle. Labeling over smooth muscle was denser in small compared to large airways. Vascular smooth muscle was not labeled in either human and guinea pig. The alveolar walls were uniformly labeled in both species. The functional significance of pulmonary peripheral-type benzodiazepine receptors remains to be detd.

IT **553-12-8**, Protoporphyrin IX
RL: BIOL (Biological study)
(peripheral benzodiazepine receptors binding to, in lung of humans and lab. animals)

RN 553-12-8 CAPLUS

CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1989:502743 CAPLUS
DOCUMENT NUMBER:	111:102743
TITLE:	Sustained-release pharmaceutical matrixes containing polymer blends having reverse phase morphology and giving a zero-order rate
INVENTOR(S):	Kashdan, David S.
PATENT ASSIGNEE(S):	Eastman Kodak Co., USA
SOURCE:	U.S., 21 pp. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 4795641	A	19890103	US 1987-87566	19870820
CA 1319468	A1	19930629	CA 1988-571672	19880711
EP 303853	A2	19890222	EP 1988-111876	19880723
EP 303853	A3	19901122		
EP 303853	B1	19930922		
R: CH, DE, FR, GB, LI				
JP 01090231	A2	19890406	JP 1988-204825	19880819

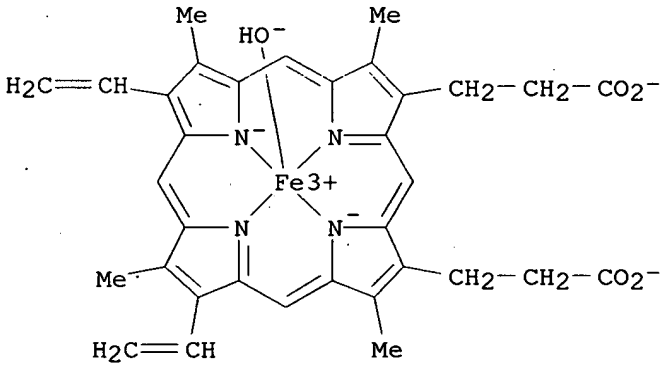
PRIORITY APPLN. INFO.: US 1987-87566 19870820

AB Disclosed are polymer blends contg. up to 40% by wt. an insol. cellulose acetate polymer (20-44% acetyl content) and >60% by wt. a sol. cellulose acetate phthalate, cellulose acetate trimellitate, and cellulose acetate succinate polymer. The blends have reverse phase morphol., i.e., wherein the sol. polymer phase comprises regions in the insol. continuous polymer phase. The blends are useful for zero-order controlled delivery of bioactive agents such as pharmaceutical and agricultural chems. Films made of a mixt. of 25% cellulose acetate (39.4% acetyl) and 75% cellulose acetate succinate, were loaded with 5, 10 or 20% dextromethorphan. At 5 and 10% loading, zero-order release was shown in simulated intestinal fluid, for 2.5 h, subsequent to an initial 5-min burst. At 20% loading, a greater burst effect was shown. Reverse-phase morphol. of the polymer matrix led to the retention of the structural integrity of the matrix after extn. of the sol. polymer.

IT **15489-90-4**
RL: BIOL (Biological study)
(stimulant agents for, sustained-release formulations contg. polymer matrix and, reverse-phase morphol. in alk. medium in relation to)

RN 15489-90-4 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]hydroxy-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)



●2 H+

L7 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1989:490303 CAPLUS

DOCUMENT NUMBER: 111:90303

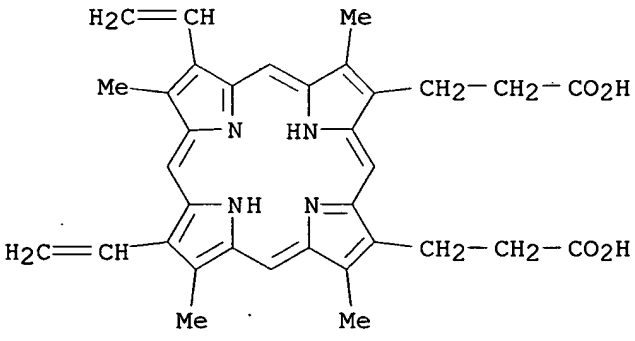
TITLE: Differential binding properties of the peripheral-type benzodiazepine ligands [3H]PK 11195 and [3H]Ro 5-4864

in trout and mouse brain membranes
AUTHOR(S): Eshleman, A. J.; Murray, T. F.
CORPORATE SOURCE: Coll. Pharm., Oregon State Univ., Corvallis, OR, USA
SOURCE: Journal of Neurochemistry (1989), 53(2), 494-502
CODEN: JONRA9; ISSN: 0022-3042
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-affinity binding sites for [3H]PK 11195 have been detected in brain membranes of rainbow trout (Salmo gairdneri) and mouse forebrain, where the densities of receptors were 1,030 and 445 fmol/mg of protein, resp. Ro 5-4864 (4'-chlorodiazepam) was 2,200-fold less potent as a competitor of [3H]PK 11195 binding in the piscine than the murine membranes. Investigation of the regional distribution of these sites in trout yielded a rank order of d. of spinal cord > olfactory bulb = optic tectum = rhombencephalon > cerebellum > telencephalon. This site in trout shared some of the characteristics of the peripheral-type benzodiazepine receptor (PTBR) (also known as the mitochondrial benzodiazepine receptor) in rodents, i.e., high affinity for PK 11195 and the endogenous ligand protoporphyrin IX, but was unique in the low affinity of Ro 5-4864 (41 .mu.M) and **diazepam** and the relatively high affinity of the calcium channel ligand diltiazem and two central benzodiazepine ligands, CGS 8216 and CGS 9896. The differential affinity for the two prototypic PTBR ligands in trout is similar to that previously obsd. in calf and human brain membranes. Structural differences for the trout sites are indicated by the relative inability of di-Et pyrocarbonate to modify histidine residues of the binding site in trout as compared with mouse membranes. Heterogeneity of binding of the two prototypic PTBR ligands in mouse brain membranes was indicated by additivity studies, equil. competition expts., and satn. isotherms, which together support the hypothesis that Ro 5-4864 discriminates between two [3H]PK 11195 binding sites having high (nanomolar) and low (micromolar) affinity, resp.

IT **553-12-8**, Protoporphyrin IX
RL: BIOL (Biological study)
(peripheral-type benzodiazepine ligand binding in trout and mouse brain membranes response to)

RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



L7 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:237136 CAPLUS

DOCUMENT NUMBER: 110:237136
TITLE: Coacervates for delivery of physiologically active substances
INVENTOR(S): Ecanow, Bernard
PATENT ASSIGNEE(S): Medaphore, Inc., USA
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 274431	A2	19880713	EP 1988-300085	19880107
EP 274431	A3	19890111		
EP 274431	B1	19940504		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4794000	A	19881227	US 1987-1814	19870108
US 4914084	A	19900403	US 1987-31237	19870326
US 4963367	A	19901016	US 1987-130550	19871215
AT 105183	E	19940515	AT 1988-300085	19880107

PRIORITY APPLN. INFO.:

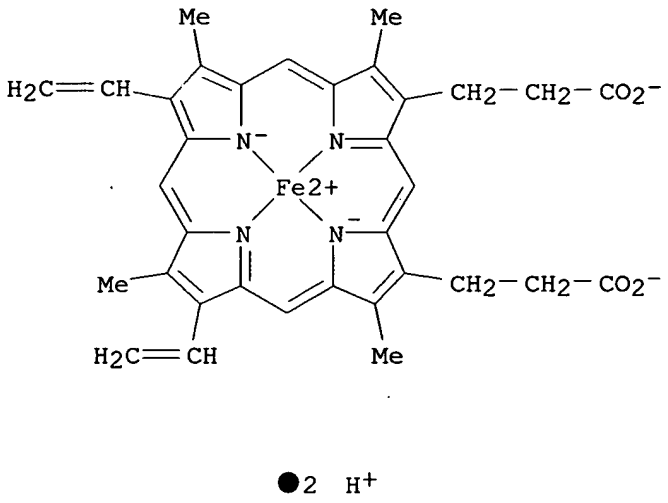
US 1987-1814	19870108
US 1987-31237	19870326
US 1987-54193	19870526
US 1987-54194	19870526
US 1987-130550	19871215
US 1984-604476	19840427
US 1984-604483	19840509
US 1984-608483	19840509
US 1985-710048	19850311
US 1985-711066	19850312
US 1985-811675	19851220
US 1986-835550	19860303
US 1986-710048	19860311
US 1986-711066	19860312
US 1986-896844	19860814
US 1987-1314	19870108
EP 1988-300085	19880107

AB Coacervates are used alone or as liposome coatings in delivery of physiol. active substances, as antiobesity agents, and as artificial blood. Lecithin 10 g and erythromycin 5 g were spray dried from CCl4 soln., and suspended in water 100 mL contg. polymd. albumin 10 and monomeric lecithin 10 g. Butanol was added dropwise and a coacervate formed and coated the particles. The particles were sepd. from the liq. and dried to give oral coacervate-coated erythromycin, which may be formed into tablets, capsules, syrups, etc.

IT **14875-96-8**
RL: PROC (Process)
(formulation of, in coacervates)

RN 14875-96-8 CAPLUS

CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H^+

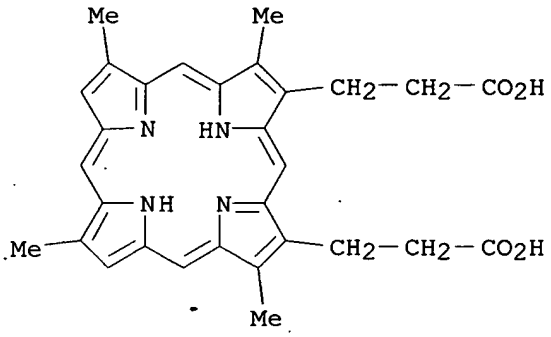
L7 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:128070 CAPLUS
DOCUMENT NUMBER: 110:128070
TITLE: Characterization of ligand binding to mitochondrial benzodiazepine receptors
AUTHOR(S): Hirsch, James D.; Beyer, Carl F.; Malkowitz, Lorraine; Loullis, Costas C.; Blume, Arthur J.
CORPORATE SOURCE: Med. Res. Div., Am. Cyanamid Co., Pearl River, NY, 10965, USA
SOURCE: Molecular Pharmacology (1989), 35(1), 164-72
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The affinity and d. of binding sites for [H]Ro5-4864 and [3H]PK11195 in intact and fragmented rat kidney mitochondria were studied. These sites are known as peripheral-type or mitochondrial benzodiazepine receptors (MBR) and they function in vitro as modulators of the mitochondrial respiratory control. In intact mitochondria, there were approx. the same no. of binding sites for [3H]PK11195 as for [3H]Ro5-4864, and their apparent Kd values were identical. However, in mitochondrial fragments, there were 80% more binding sites for [3H]Ro5-4864 than for [3H]PK11195. Rat kidney mitochondria were fractionated by decompression and digitonin-based methods into outer and inner membrane-contg. fractions before and after incorporation of the MBR-specific photoaffinity ligand [3H]PK14105. Assays of selective mitochondrial membrane markers and [3H]Ro5-4864 binding or specifically bound [3H]PK14105 revealed that the receptors were found in the mitochondrial outer membrane. The binding of a large no. of structurally and pharmacol. diverse compds. to MBR were examd. by studying their ability to inhibit the binding of both 3H-ligands. These compds. had affinities ranging 0.015-100 .mu.M and, with a few exceptions, were similar in their abilities to bind to MBR in intact and fragmented mitochondria. However, there was considerable variation in the ratios between drug potencies at displacing [3H]Ro5-4864 and [3H]PK11195. This represents a new form of evidence that these 2 radioligands do not label identical sites on the receptor. Thirteen of the drugs, including [H]Ro5-4864 and [H]PK11195, were analyzed as to the nature of the inhibition and, with only 2 exceptions, were competitive

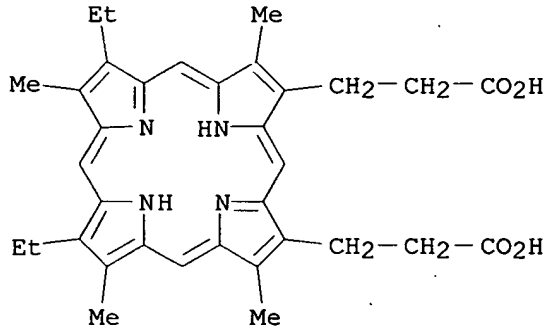
inhibitors. One drug, Konig's polyanion, was uncompetitive whereas the other, cyclosporin A, was a noncompetitive inhibitor. These studies revealed several new classes of MBR ligands and suggest that the relationship between ligand structure and binding affinity is highly complex.

IT **448-65-7**, Deuteroporphyrin IX **493-90-3**, Mesoporphyrin IX **531-14-6** **553-12-8**, Protoporphyrin IX **16009-13-5**, Hemin
RL: BIOL (Biological study)
(peripheral-type benzodiazepine receptor of mitochondria binding by, structure in relation to)

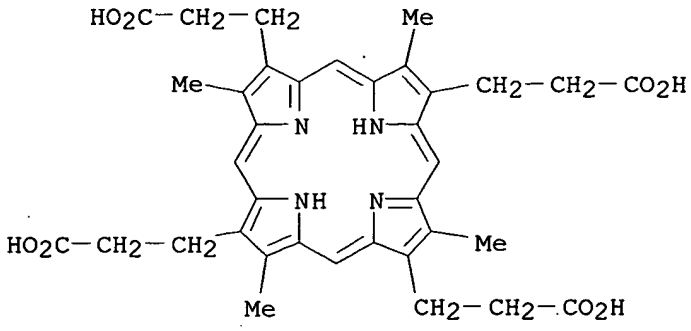
RN 448-65-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- (9CI) (CA INDEX NAME)



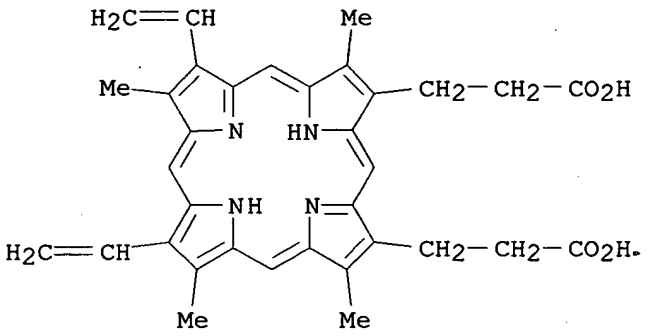
RN 493-90-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



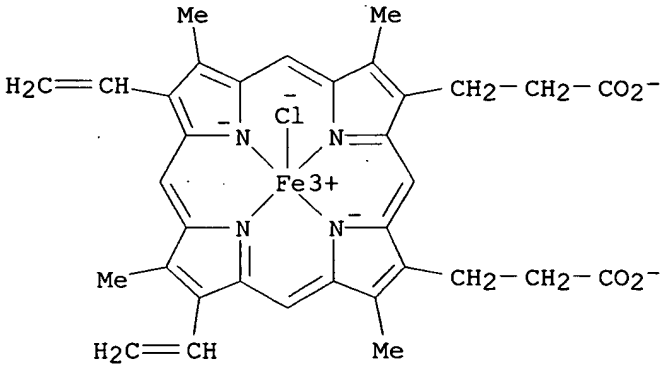
RN 531-14-6 CAPLUS
CN 21H,23H-Porphine-2,7,12,17-tetrapropanoic acid, 3,8,13,18-tetramethyl- (9CI) (CA INDEX NAME)

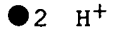


RN 553-12-8 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (9CI) (CA INDEX NAME)



RN 16009-13-5 CAPLUS
CN Ferrate(2-), chloro[7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)



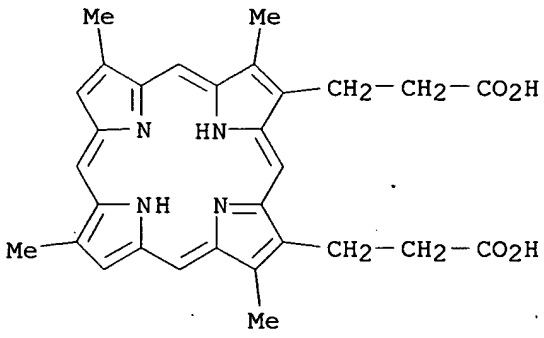


L7 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:108099 CAPLUS
DOCUMENT NUMBER: 110:108099
TITLE: Mitochondrial benzodiazepine receptors mediate inhibition of mitochondrial respiratory control
AUTHOR(S): Hirsch, James D.; Beyer, Carl F.; Malkowitz, Lorraine; Beer, Bernard; Blume, Arthur J.
CORPORATE SOURCE: Med. Res. Div., Am. Cyanamid Co., Pearl River, NY, 10965, USA
SOURCE: Molecular Pharmacology (1989), 35(1), 157-63
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Drugs that bound to the peripheral-type or mitochondrial benzodiazepine receptors in rat kidney mitochondria produced several effects on mitochondrial respiration with succinate and malate/pyruvate as substrates. These drugs increased state IV and decreased state III respiration rates, which resulted in a decrease in the respiratory control ratio. ADP:O ratios were not affected. The receptor binding affinities of a set of 10 compds. (Ro 5-4864, PK11195, **diazepam**, mesoporphyrin IX, flunitazepam, deuteroporphyrin IX, dipyridamole, di-Bu phthalate, cyclosporin A, and CL259,763) correlated over a concn. range of almost 4 orders of magnitude with their potencies at inhibiting respiratory control. The anxiolytic benzodiazepine clonazepam had no effect on mitochondrial respiratory control and bound with negligible affinity to the receptor. The magnitude of the effect of Ro 5-4865 on respiration increased in parallel with the d. of mitochondrial benzodiazepine receptors in mitochondria from liver, kidney, and adrenal. Thus, ligand binding to mitochondrial benzodiazepine receptors seems to result in inhibition of mitochondrial respiratory control. This effect may help to explain the pleiotropic effects of receptor ligands on intact cells.

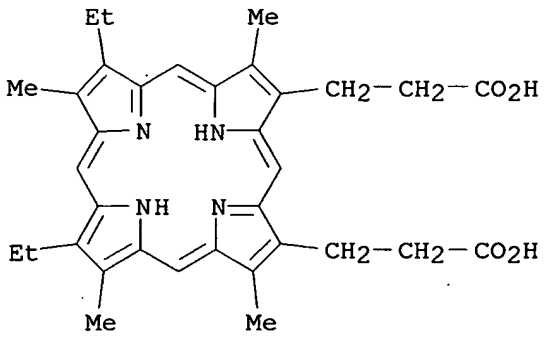
IT **448-65-7**, Deuteroporphyrin IX **493-90-3**, Mesoporphyrin IX
RL: BIOL (Biological study)
(mitochondrial respiration response to)

RN 448-65-7 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- (9CI) (CA INDEX NAME)

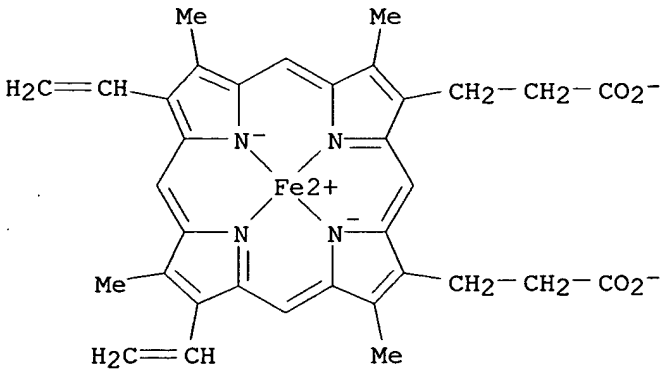


RN 493-90-3 CAPLUS
CN 21H,23H-Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-

(9CI) (CA INDEX NAME)



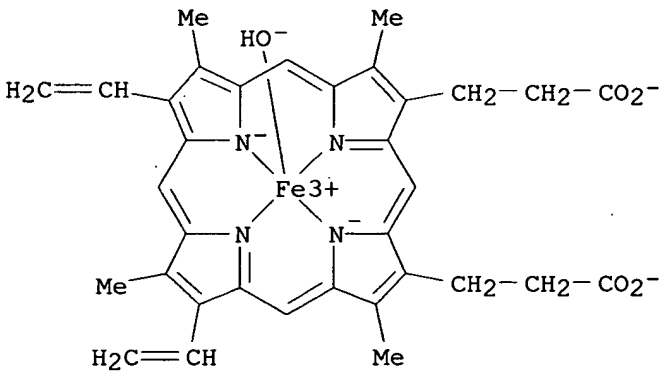
L7 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:564805 CAPLUS
DOCUMENT NUMBER: 105:164805
TITLE: Effect of N-piperazinylmethyl-3,3-diethyl-2,4-pyridinedione on liver drug metabolizing enzyme systems
AUTHOR(S): Belcheva, I.; Kadiiska, M.; Alov, P.; Stoichev, Ts.
CORPORATE SOURCE: Inst. Physiol., Sofia, Bulg.
SOURCE: Doklady Bolgarskoi Akademii Nauk (1986), 39(4), 91-4
CODEN: DBANAD; ISSN: 0366-8681
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Like phenobarbital, N-piperazinylmethyl-3,3-diethyl-2,4-pyridinedione (I) [80733-97-7] given s.c. to rats for 3 days at high doses (50% of the LD50) increased only the activity of ethylmorphine-N-demethylase [9032-78-4] of the liver microsomal enzyme system. In contrast to phenobarbital, I did not increase cytochrome P 450 [9035-51-2] and microsomal heme [**14875-96-8**] contents. I or **diazepam** when given s.c. to rats repeatedly for 10 days at seizure-suppressing doses did not induce the liver drug-metabolizing enzyme systems.
IT **14875-96-8**
RL: BIOL (Biological study)
(of liver microsome, piperazinylmethyldiethylpyridinedione effect on)
RN 14875-96-8 CAPLUS
CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



L7 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:539286 CAPLUS
DOCUMENT NUMBER: 103:139286
TITLE: Hematin and bilirubin binding to human serum albumin and newborn serum
AUTHOR(S): Ho, C. K.; Robertson, A. F.; Karp, W. B.
CORPORATE SOURCE: Dep. Pediatr., Med. Coll. Georgia, Augusta, GA, 30912, USA
SOURCE: Acta Paediatrica Scandinavica (1985), 74(3), 372-7
CODEN: APSVAM; ISSN: 0001-656X
DOCUMENT TYPE: Journal
LANGUAGE: English

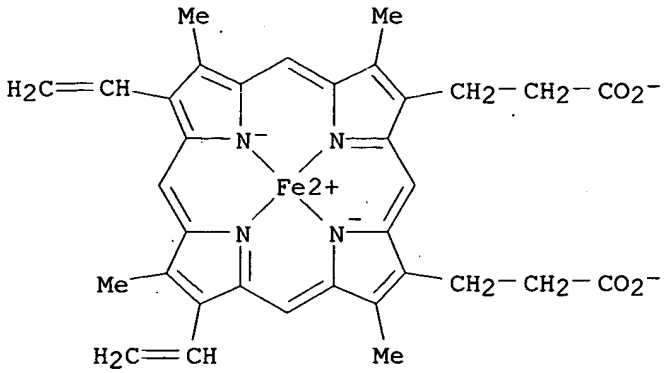
AB The effect of hematin on bilirubin-albumin binding was studied using the peroxidase assay and a light-scattering technique for measuring unbound bilirubin. The results showed that hematin does not affect bilirubin-albumin binding in human newborn blood serum. To det. if other albumin binding functions are affected by hematin, a microdialysis rate technique was used employing 2 ligands, **diazepam** and monoacetyldiaminodiphenyl sulfone (I). Hematin did not utilize the **diazepam** binding function of albumin, but did decrease albumin binding of I. Hence, the I and bilirubin binding functions are not identical. The clin. usefulness of reserve albumin equiv detn. using I is discussed.

IT **15489-90-4**
RL: BIOL (Biological study)
(bilirubin binding by albumin of human newborn blood serum response to)
RN 15489-90-4 CAPLUS
CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]hydroxy-, dihydrogen, (SP-5-13)- (9CI) (CA INDEX NAME)



●2 H^+

L7 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1976:38899 CAPLUS
DOCUMENT NUMBER: 84:38899
TITLE: Heme catabolism during short-term treatment with phenobarbital, **diazepam**, and oxazepam
AUTHOR(S): Mercke, C.; Cavallin-Stahl, E.; Lundh, B.
CORPORATE SOURCE: Dep. Med., Univ. Hosp., Lund, Swed.
SOURCE: Acta Medica Scandinavica (1975), 198(3), 149-54
CODEN: AMSVAZ; ISSN: 0001-6101
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB No change in CO prodn. (VCO), total body heme [**14875-96-8**] (TBH) or serum bilirubin [635-65-4] (SB) were obsd. in healthy young men after 100 mg phenobarbital (I) [50-06-6] (10 subjects), 15 mg **diazepam** [439-14-5] (7 subjects) and 75 mg oxazepam [604-75-1] (7 subjects), resp., daily for 7 days. However, when the pooled postdrug data were compared with the pooled baseline values, mean VCO showed a probably significant increase from 12.6 to 14.7 .mu.mole/mmole TBH and day. Thus, although I is known to increase the hepatic heme turnover, this effect is not measurable in terms of total heme turnover, no more than 20% of which comes from the liver.
IT **14875-96-8**
RL: BIOL (Biological study)
(catabolism of, drugs effect on)
RN 14875-96-8 CAPLUS
CN Ferrate(2-), [7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-2,18-dipropanoato(4-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, dihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)



●2 H^+

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	335.09	483.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-46.87	-46.87

STN INTERNATIONAL LOGOFF AT 10:27:23 ON 14 MAY 2003